

# Bridging the gap between rooted and unrooted phylogenetic networks

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## Abstract

The need for structures capable of accommodating complex evolutionary signals such as those found in, for example, wheat has fueled research into phylogenetic networks. Such structures generalize the standard phylogenetic tree model by also allowing cycles and have been introduced in rooted and unrooted form. In contrast to phylogenetic trees, however, surprisingly little is known about the interplay between both types thus hampering our ability to make much needed progress for rooted phylogenetic networks by drawing on insights from their much better understood unrooted counterparts. Unrooted phylogenetic networks are underpinned by split systems and by focusing on them we establish a first link between both types. More precisely, we develop a link between 1-nested phylogenetic networks which are examples of rooted phylogenetic networks and the well-studied median networks (aka Buneman graph) which are examples of unrooted phylogenetic networks. In particular, we show that not only can a 1-nested network be obtained from a median network but also that that network is, in a well-defined sense, optimal. Along the way, we characterize circular split systems in terms of the novel  $\mathcal{I}$ -intersection closure of a split system and establish the 1-nested analogue of the fundamental “Splits Equivalence Theorem” for phylogenetic trees.

*Keywords:* phylogenetic network, Buneman graph, circular split system, closure, median network

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## 1. Introduction

A widely accepted evolutionary scenario for some economically important crop plants such as wheat is that their evolution has been shaped by complex reticulate processes [26]. The need for structures capable of representing

the telltale signs left behind by them has fueled research into phylogenetic networks which generalize the commonly used phylogenetic tree model for studying molecular evolution (see Fig 1 for examples and Section 2 for formal definitions). However, despite many years of research into phylogenetic networks (see e.g. the graduate text books [20, 22]) important questions concerning their structure have remained unanswered so far (see e.g. [18]).

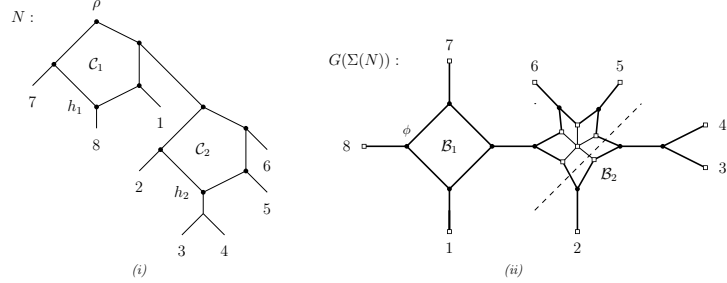


Figure 1: (i) A rooted phylogenetic network in the form of a level-1 network  $N$  on  $X = \{1, \dots, 8\}$ . The root is labeled by  $\rho$ , all edges are directed downwards, and vertices  $h_1$  and  $h_2$  represent hypothesised reticulate evolutionary events. (ii) An unrooted phylogenetic network on  $X$  in the form of a median network on the split system induced by the underlying graph of  $N$ . The dashed line indicates the split  $234|15678$  – see text for details.

Mimicking the situation for phylogenetic trees which can either be rooted or unrooted, phylogenetic networks have been introduced in terms of rooted directed acyclic graphs whose outdegree zero vertices correspond to the taxa (e.g. species) of interest and also in terms of representations of *splits systems*, that is, collections of bipartitions of the taxa set in question. In general, the former seem more attractive as they allow the inclusion of directionality and thus readily lend themselves to an interpretation within an evolutionary context. However, they suffer from the fact that they are generally poorly understood from a combinatorial point of view thus hampering our ability to design powerful reconstruction algorithms for them. Unrooted counterparts of rooted phylogenetic networks include the popular NeighborNet approach [11] as well as median networks [5, 7] (sometimes also called *Buneman graphs* – see e.g. [16]) and related structures (see e.g. [3, 4]) and the methodology underpinning them is far more advanced. This is in part due to a rich body of literature surrounding such graphs which have appeared under various guises such as co-pair hypergraphs [8, 9] and have been studied in terms of median algebras [6], 1-skeletons of  $CAT(0)$  cubical complexes [2], retracts of hypercubes [1], sets of solutions of 2-SAT formulas [6], tight spans of metric spaces (see e.g. [15] and also the more recent text book [14] and the references therein), and S2 binary convexities [31] (see also [25] for a review of median graphs). In an independent line of research, numerous deep results have also been obtained for the special case that the (unrooted) phylogenetic network is in fact a tree (see e.g. [29, 14]).

From a combinatorial point of view, rooted and unrooted phylogenetic trees

can be thought of as certain *cluster systems* (i. e. collections of non-empty subsets of the tree's leaf set) and split systems, respectively, and the Farris Transform allows one to readily translate between both by ignoring/identifying a root vertex and edge-directions (see e. g. [14] for details). As it turns out, the more general rooted and unrooted phylogenetic networks also induce cluster systems and split systems, respectively. Thus, it is conceivable that a similar strategy could be used to foster our understanding of rooted phylogenetic networks. For this to work however, some care needs to be taken since the graph obtained from a rooted phylogenetic network by ignoring its root and edge-directions can contain odd length cycles and thus is not a (splits based) phylogenetic network as the inner workings of such network require them to only contain cycles of even length.

Intriguingly, any rooted phylogenetic network  $N$  also induces a split system  $\Sigma(N)$  by taking minimal edge cuts in the *underlying graph*  $U(N)$  of  $N$  i. e. the graph obtained from  $N$  by ignoring edge directions and suppressing the root in case its out-degree in  $N$  is two (see [10] and also [17]). Such graphs can be thought of as intermediate steps between rooted and unrooted phylogenetic networks and although they do not contain directionality information they still provide valuable information on the number of reticulate evolutionary events which is a difficult problem of interest in its own right. Furthermore,  $\Sigma(N)$  can also be represented in terms of an unrooted phylogenetic network (although the way  $\Sigma(N)$  is displayed by such a network is fundamentally different from the way  $\Sigma(N)$  is displayed by  $N$  – see Figs 1 and 2 for an illustration of this fact in terms of the Buneman graph  $G(\Sigma(N))$  associated to  $\Sigma(N)$  where the way the split  $234|15678$  is displayed by  $N$  and  $G(\Sigma(N))$  is indicated in terms of a dashed line).

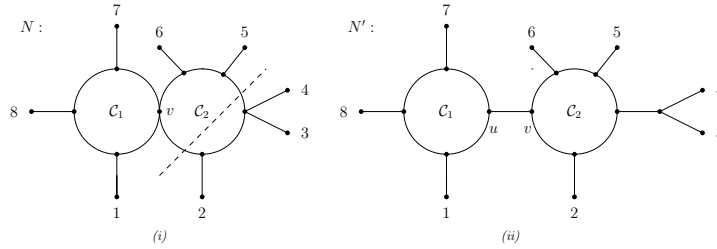


Figure 2: (i) A 1-nested network for which the induced split system is  $\Sigma(N')$ . As in Fig. 1, the dashed line indicates the split  $234|15678$  (ii) The underlying graph of the rooted level-1 network  $N$  depicted in Fig. 1.

In general, the split system induced by a rooted phylogenetic network  $N$  on some set  $X$  can be very complicated. However, in case  $N$  is level-1 [23, 24] which essentially means that no two cycles in  $U(N)$  share a vertex then the induced split system  $\Sigma(N)$  is *circular* (i. e. the elements of  $X$  can be arranged around a cycle  $C$  so that the split system induced on  $X$  by deleting any two edges of  $C$  contains in  $\Sigma(N)$ ) [17]. This property is central to the aforementioned popular

NeighborNet approach and particularly attractive as it guarantees any such split system to be representable in the plane in terms of an unrooted phylogenetic networks without crossing edges.

Level-1 networks and also the more general rooted 1-nested networks (i. e. the networks obtained by replacing the requirement of vertex disjointness between cycles in the underlying graph in the definition of a level-1 network by allowing cycles to share at most one vertex – see [28]) have attracted a considerable amount of attention in the literature (see e. g. [21] and the references therein). For ease of readability and also reflecting the fact that the focus of this paper lies on understanding split systems induced by rooted level-1 networks we will from now on, unless indicated otherwise, refer to the underlying graph of a rooted 1-nested network as a 1-nested network.

As is easy to see, any circular split system on some set  $X$  can be represented in terms of a level-1 network  $N$  on  $X$  by taking the unique cycle of  $N$  to be the aforementioned cycle  $C$ , attaching to each vertex  $v$  of  $C$  a pendant edge  $e$  and shifting the element of  $X$  labelling  $v$  to the degree one vertex of  $e$ . Although structurally very simple, these types of networks are of interest in their own right as they are special types of so called unicyclic networks [30] (see also [27] for a biological example) which have been related to the tree arrangement problem in [30]. However, as the level-1 network depicted in Fig. 2(ii) indicates for the split system  $\Sigma$  comprising of all splits of the form  $x|X - x^1$  where  $x \in X := \{1, \dots, 8\}$  and the splits  $81|234567$ ,  $78|123456$ ,  $781|23456$ ,  $234|56781$ ,  $34|567812$ ,  $345|67812$ ,  $2345|6781$ ,  $3456|7812$  and  $56|78123$ , the resulting level-1 network is generally not optimal as it displays a total of  $\binom{|X|}{2}$  distinct splits of  $X$  whereas the level-1 network  $N$  depicted in that figure also displays all splits of  $\Sigma$  and postulates fewer additional splits. Furthermore, the 1-nested network pictured in Fig. 2(i) also displays  $\Sigma$  and so does the subgraph in terms of bold edges of the Buneman graphs  $G(\Sigma)$  pictured Fig. 1(ii).

As it turns out, this is not a coincidence since Theorem 5.5 combined with Corollary 4.8 ensures that, up to isomorphism and a mild condition, the network obtained from the Buneman graph pictured in Fig. 1(ii) by deleting the central vertex in  $\mathcal{B}_2$ , its incident edges and suppressing the resulting degree two vertices is in fact optimal. Corollary 4.8 itself may be the 1-nested analogue of the fundamental “Splits Equivalence Theorem” for unrooted phylogenetic trees [29, Theorem 3.1.4] and is a consequence of Theorem 4.7. The purpose of that theorem is to establish that the novel  $\mathcal{I}$ -intersection closure of a split system  $\Sigma$  can be used to obtain a 1-nested network  $N$  whose induced split system  $\Sigma(N)$  does not only contains  $\Sigma$  but is also minimum. Given that a closure is not known for rooted phylogenetic networks it might be interesting to see if our closure could be used to this effect (see also Section 6).

As an important stepping stone for establishing Theorem 4.7, we charac-

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<sup>1</sup>For ease of readability, we represent a split  $\{A, B\}$  of a set  $X$  as  $A|B$  where the order of  $A$  and  $B$  is irrelevant. Also if  $A = \{x_1, \dots, x_k\}$  and  $B = \{x_{k+1}, \dots, x_n\}$  for some  $1 \leq k \leq n-1$  we write  $x_1 \dots x_k | x_{k+1} \dots x_n$  rather than  $\{x_1, \dots, x_k\} | \{x_{k+1}, \dots, x_n\}$ .

terize split systems that are induced by a 1-nested network in terms of their  $\mathcal{I}$ -intersection closure (Theorem 3.6) and also when a circular split system that is  $\mathcal{I}$ -intersection closed is (set-inclusion) maximal (Theorem 4.5). We remark in passing that Theorem 4.7 complements a result by Dinitz and Nutov [13, 12] who characterized split systems that can be represented by 1-nested networks in terms of “crossings” and “cactus models” and a result by Brandes and Cornelsen [10] who gave an  $\mathcal{O}(f + |X| + |\Sigma|)$  algorithm for deciding if a split system  $\Sigma$  on  $X$  can be represented by a 1-nested network or not and if so constructing such a network where  $f \leq |X| \times |\Sigma|/2$ . Since it is not difficult to see that crossing split systems are a particular type of split system that is  $\mathcal{I}$ -intersection closed their result is viewable as a consequence.

The outline of the paper is as follows. In the next section we introduce some relevant basic terminology such as level-1 and 1-nested network. In Section 3, we introduce and study the  $\mathcal{I}$ -closure operation which lies at the heart of Theorem 3.6. In Section 4, we turn our attention to (set-inclusion) maximal circular split systems and establish Theorems 4.5 and 4.7. As part of this, we characterize such collections in terms of a property of the incompatibility graph of a split system which we define in that section. Using insights into the structure of the Buneman graph presented in [16], we establish Theorem 5.5 in Section 5. We conclude with some open problems in Section 6.

## 2. Preliminaries

In this section, we present relevant basic definitions concerning splits and phylogenetic networks. Throughout the paper, we assume that  $X$  is a finite set with  $n \geq 3$  elements and that, unless stated otherwise, split systems are non-empty.

### 2.1. Splits and split systems

For all subsets  $A \subseteq X$ , we put  $\bar{A} = X - A$ . Furthermore, for all elements  $x \in X$  and all splits  $S$  of  $X$ , we denote by  $S(x)$  the element of  $S$  that contains  $x$ . The *size* of a split  $A|B$  is defined as  $\min\{|A|, |B|\}$  and a split  $S$  is called *trivial* if its size is one. Two splits  $S_1$  and  $S_2$  of  $X$  are called *compatible* if there exists some  $A_1 \in S_1$  and some  $A_2 \in S_2$  such that  $A_2 \subsetneq A_1$  and *incompatible* otherwise. More generally, a split system  $\Sigma$  on  $X$  is called *compatible* if any two splits in  $\Sigma$  are compatible and *incompatible* otherwise.

Suppose  $x_1, x_2, \dots, x_n, x_{n+1} := x_1$  is a circular ordering of the elements of  $X$  (where we take indices modulo  $n$ ). Then for all  $i, j \in \{1, \dots, n\}$  we call the subsequence  $x_i, x_{i+1}, \dots, x_j$  the *interval* from  $x_i$  to  $x_j$  and denote it by  $[x_i, x_j]$ . We say that a split system  $\Sigma$  on  $X$  is *circular* if there exists a circular ordering  $x_1, x_2, \dots, x_n, x_{n+1} = x_1$  of the elements of  $X$  such that for every split  $S = A|B \in \Sigma$  there exists an  $i, j \in \{1, \dots, n\}$  such that  $A = [x_i, x_j]$  and  $B = [x_{j+1}, x_{i-1}]$ . Note that there are  $(n-1)!$  circular orderings for  $X$  and that a circular split system on  $X$  has size at most  $n(n-1)/2$ .

## 2.2. Phylogenetic networks

Suppose  $G$  is a simple connected graph. Then the *cyclomatic number* of  $G$  is the minimum number of edges that need to be removed from  $G$  to obtain a tree. A *cut-edge* of  $G$  is an edge  $e$  whose removal disconnects  $G$ . We call  $e$  *trivial* if it is incident to a *leaf*  $v$  of  $G$ , that is, the degree of  $v$  is one.

We call a simple connected graph  $N$  a *phylogenetic network (on  $X$ )* if  $X$  is the set of leaves of  $N$ , every other vertex has degree at least three, and every cycle has length at least four. The reason for the latter requirement is that a cycle of length three displays the same split system as the star tree with three leaves (but not the same multi-set of splits) which is undesirable from a uniqueness point of view. As for rooted phylogenetic networks, we call a phylogenetic network  $N$  *simple* if all cut-edges of  $N$  are trivial, *level-1* if every vertex but the leaves have degree three and the maximum cyclomatic number of the bridgeless connected components of  $N$  is one [17], and, inspired by [28], *1-nested* if  $N$  can be obtained from a level-1 network by collapsing (non-trivial) cut-edges. For example, the graph  $N'$  depicted in Fig. 2(i) is a level-1 network on  $X = \{1, \dots, 8\}$  and the graph pictured in Fig. 2(ii) is a 1-nested network on  $X$  as it can be obtained from  $N'$  by collapsing the edge  $\{u, v\}$ .

Finally, we say that two phylogenetic networks  $N$  and  $N'$  on  $X$  are *isomorph* if there exists a graph isomorphism between  $N$  and  $N'$  that is the identity on  $X$ .

## 2.3. Displaying splits

Suppose that  $N$  is a phylogenetic network on  $X$ . Then we say that a split  $S = A|B$  of  $X$  is *displayed* by  $G$  if there exists a set-inclusion minimal cut of  $G$ , that is, a set  $E_S$  of edges of  $G$  such that the deletion of the edges in  $E_S$  disconnects  $G$  into two connected components, one of whose set of leaves is  $A$  and the other is  $B$ . More generally, we say that a split system  $\Sigma$  is *displayed* by  $N$  if every split of  $\Sigma$  is displayed by  $N$ , that is,  $\Sigma \subseteq \Sigma(N)$ . Also, we say that a split  $S \in \Sigma(N)$  is *displayed by a cycle  $C$*  of  $N$  if  $E_S$  is contained in the edge set of  $C$ .

Note that in case  $N$  is a 1-nested network and  $S \in \Sigma(N)$  then  $|E_S| \in \{1, 2\}$ . Furthermore, note that if  $e = \{u, v\}$  is the unique element in  $E_S$  and neither  $u$  nor  $v$  is contained in a cycle of  $N$  then  $e$  must be a cut-edge of  $N$  and the multiplicity of the split  $S_e$  induced by deleting  $e$  is one. Note also that if  $e = \{u, v\}$  is a cut-edge of  $N$  where  $u$  or  $v$  is contained in a cycle  $C$  of  $N$ , say  $u$ , then  $S_e$  is also induced by deleting the edges of  $C$  incident with  $u$ . Thus, the multiplicity of a split induced by a 1-nested network can either be one, two, or three. We call a split  $S$  of multiplicity two or more in a maximal partial-resolution of  $N$  an *m-split* of  $N$  (or more precisely of  $C$  if  $C$  is the cycle of  $N$  that displays  $S$ ). Finally, note that the split system induced by a 1-nested network  $N$  on  $X$  is the same as the resolution of  $N$  to a 1-nested network by repeatedly applying the following two replacement operations (and their complements which we denote by (R1') and (R2'), respectively):

- (R1) a vertex  $v$  of a cycle of  $N$  incident with  $l \geq 2$  non-cycle edges  $e_1, \dots, e_l$  is replaced by an edge one of whose vertices is  $v$  and the other is incident with  $e_1, \dots, e_l$  and vice versa, and
- (R2) a cut-vertex  $v$  shared by two cycles  $C_1$  and  $C_2$  is replaced by a cut-edge one of whose vertices is contained in  $C_1$  and the other in  $C_2$ .

However, the multi-sets of splits induced by both networks are clearly different. We call the vertex  $v$  in (R1) or (R2) *partially-resolved*. More generally, we call a 1-nested network  $N'$  a *partial-resolution* of a 1-nested network  $N$  if  $N'$  can be obtained from  $N$  by partially resolving vertices of  $N$ . Moreover, we call a partial-resolution  $N'$  of  $N$  a *maximal partial-resolution* of  $N$  if the only way to obtain a partial-resolution of  $N'$  is to apply (R1') or (R2'). In this case, we also call  $N'$  *maximal partially-resolved*.

To illustrate some of these definitions consider the 1-nested network  $N$  on  $X = \{1, \dots, 8\}$  depicted in Fig. 2(i). Then, the splits  $7|X - \{7\}$ ,  $8|X - \{8\}$ ,  $1|X - \{1\}$  and  $781|23456$  are displayed by  $N$ . In fact, they are m-splits for the cycle  $C_1$  of  $N$ . Furthermore,  $N'$  is a partial-resolution of  $N$  and  $\Sigma(N)$  only contains splits of multiplicity one or two.

### 3. Characterizing of 1-nested networks in terms of $\mathcal{I}$ -intersections

In this section, we introduce and study the  $\mathcal{I}$ -intersection closure of a split system which turns out to be key for our characterization of 1-nested networks in terms of split systems which we present in Theorem 3.6. We start with introducing the concept of an intersection between splits.

Suppose  $S_1$  and  $S_2$  are two distinct splits of  $X$  and  $A_i \in S_i$ ,  $i = 1, 2$ , such that  $A_1 \cap A_2 \neq \emptyset$ . Then we call the split  $A_1 \cap A_2 | \bar{A}_1 \cup \bar{A}_2$  of  $X$  associated to  $\{S_1, S_2\}$  an *intersection of  $S_1$  and  $S_2$  (with respect to  $A_1$  and  $A_2$ )*. We denote the set of all splits obtained by taking intersections of  $S_1$  and  $S_2$  by  $\text{int}(S_1, S_2)$  and write  $\text{int}(S_1, S_2)$  rather than  $\text{int}(\{S_1, S_2\})$ . Furthermore, if  $S_1$  and  $S_2$  are incompatible then we refer to the intersection of  $S_1$  and  $S_2$  as *incompatible intersection*, or  *$\mathcal{I}$ -intersection* for short, and denote it by  $\iota(S_1, S_2)$  rather than  $\text{int}(S_1, S_2)$ .

Clearly, if  $S_1$  and  $S_2$  are compatible then  $|\text{int}(S_1, S_2)| = 3$  and  $S_1, S_2 \in \text{int}(S_1, S_2)$ . However, if  $S_1$  and  $S_2$  are incompatible then  $\iota(S_1, S_2)$  is compatible and of size four,  $S_1, S_2 \notin \iota(S_1, S_2)$ , and every split in  $\iota(S_1, S_2)$  is compatible with  $S_1$  and  $S_2$ . See Fig. 3 an illustration.

Fig. 3 suggests that every split in  $\iota(S_1, S_2)$  is displayed by the same cycle that displays  $S_1$  and  $S_2$ . That this is indeed the case is the purpose of Proposition 3.3. To state it in its full generality we next associate to a split system  $\Sigma$  of  $X$  the *intersection closure*  $\text{Int}(\Sigma)$  of  $\Sigma$ , that is,  $\text{Int}(\Sigma)$  is a (set-inclusion) minimal split system that contains  $\Sigma$  and is closed by intersection. For example, for  $\Sigma = \{12|345, 23|451\}$  we have  $\text{Int}(\Sigma) = \Sigma \cup \{1|2345, 2|3451, 3|4512, 13|452, 123|45\}$ .

We start our analysis of  $\text{Int}(\Sigma)$  with remarking that  $\text{Int}(\Sigma)$  is indeed a closure, that is,  $\text{Int}(\Sigma)$  trivially satisfies the following three properties

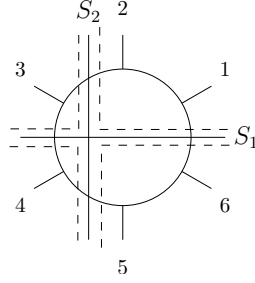


Figure 3: For a simple level-1 network on  $\{1, \dots, 6\}$  we depict the splits  $S_1$  and  $S_2$  in terms of two straight bold lines and the four splits that make up  $\iota(S_1, S_2)$  in terms of four dashed lines.

(C1)  $\Sigma \subseteq \text{Int}(\Sigma)$ .

(C2)  $\text{Int}(\text{Int}(\Sigma)) = \text{Int}(\Sigma)$ .

(C3) If  $\Sigma'$  is a split system on  $X$  for which  $\Sigma \subseteq \Sigma'$  holds then  $\text{Int}(\Sigma) \subseteq \text{Int}(\Sigma')$ .

The proof of the next lemma is a straight forward consequence of our definitions.

**Lemma 3.1.** *Suppose  $S_1$ ,  $S_2$ , and  $S_3$  are three splits on  $X$ , such that both  $\{S_1, S_2\}$  and  $\{S_2, S_3\}$  are incompatible. Then there exists at least two splits in  $\iota(S_1, S_2)$  that are incompatible with  $S_3$ .*

The next lemma implies that the intersection closure of a split system is well-defined.

**Lemma 3.2.** *Suppose  $\Sigma$  is a split system on  $X$  and  $\Sigma'$  is a further (set-inclusion) minimal superset of  $\Sigma$  that is closed by intersection. Then  $\Sigma' = \text{Int}(\Sigma)$  must hold.*

*Proof.* Since  $\Sigma'$  contains  $\Sigma$  and is intersection closed we can obtain  $\Sigma'$  via a (finite) sequence  $\Sigma = \Sigma_0 \subsetneq \Sigma_1 \subsetneq \Sigma_2 \subsetneq \dots \subsetneq \Sigma_k = \Sigma'$ ,  $k \geq 1$ , of split systems  $\Sigma_i$  such that, for all  $1 \leq i \leq k$ ,  $\Sigma_i := \Sigma_{i-1} \cup \iota(P_i)$  where  $P_i$  is a 2-set contained in  $\Sigma_{i-1}$  and  $\iota(P_i)$  is not contained in  $\Sigma_{i-1}$ . We show by induction on  $i$  that  $\Sigma_i \subseteq \text{Int}(\Sigma)$  holds.

Clearly, if  $i = 0$  then  $\Sigma_0 = \Sigma$  is contained in  $\text{Int}(\Sigma)$ . So assume that  $\Sigma_i \subseteq \text{Int}(\Sigma)$  holds for all  $1 \leq i \leq r$ , for some  $1 \leq r \leq k$ , and that  $\Sigma_r$  is obtained from  $\Sigma_{r-1}$  by intersection of two splits  $S_1, S_2 \in \Sigma_{r-1}$ . Since, by induction hypothesis,  $\Sigma_{r-1} \subseteq \text{Int}(\Sigma)$  it follows that  $S_1$  and  $S_2$  are contained in  $\text{Int}(\Sigma)$ . Since  $\text{Int}(\Sigma)$  is intersection-closed,  $\iota(S_1, S_2) \subseteq \text{Int}(\Sigma)$  follows. Hence,  $\Sigma_r = \Sigma_{r-1} \cup \iota(S_1, S_2) \subseteq \text{Int}(\Sigma)$ , as required. By induction, it now follows that  $\Sigma' \subseteq \text{Int}(\Sigma)$ . Reversing the roles of  $\Sigma'$  and  $\text{Int}(\Sigma)$  in the previous argument implies that  $\text{Int}(\Sigma) \subseteq \Sigma'$  holds too which implies  $\Sigma' = \text{Int}(\Sigma)$ .  $\square$



We remark in passing that similar arguments as the ones used in the proof of Lemma 3.2 also imply that the  $\mathcal{I}$ -intersection closed (set-inclusion) minimal superset  $\mathcal{I}(\Sigma)$  of a split system  $\Sigma$  is also well-defined (and obviously satisfies Properties (C1) – (C3)). We will refer to  $\mathcal{I}(\Sigma)$  as  $\mathcal{I}$ -intersection closure of  $\Sigma$ .

We next turn our attention to the  $\mathcal{I}$ -intersection closure of a split systems induced by a 1-nested network.

**Proposition 3.3.** *Suppose  $N$  is a 1-nested network on  $X$  and  $S_1$  and  $S_2$  are two incompatible splits contained in  $\Sigma(N)$ . Then  $\iota(S_1, S_2) \subseteq \Sigma(N)$ .*

*Proof.* Note first that two splits  $S$  and  $S'$  induced by a 1-nested network are incompatible if and only if they are displayed by pairs of edges in the same cycle  $C$  of  $N$ . For  $i = 1, 2$ , let  $\{e_i, e'_i\}$  denote the edge set whose deletion induces the split  $S_i$ . Then since  $S_1$  and  $S_2$  are incompatible, we have  $\{e_1, e'_1\} \cap \{e_2, e'_2\} = \emptyset$  and none of the connected components of  $N$  obtained by deleting  $e_i$  and  $e'_i$  contains both  $e_j$  and  $e'_j$ , for all  $i, j \in \{1, 2\}$  distinct. Without loss of generality, we may assume that when starting at edge  $e_1$  and moving clockwise through  $C$  we first encounter  $e_2$ , then  $e'_1$  and, finally  $e'_2$  before returning to  $e_1$ . Then it is straight forward to see that a split in  $\iota(S_1, S_2)$  is displayed by one of the edge sets  $\{e_1, e_2\}$ ,  $\{e_2, e'_1\}$ ,  $\{e'_1, e'_2\}$ , and  $\{e'_2, e_1\}$ . Thus,  $\iota(S_1, S_2) \subseteq \Sigma(N)$ .  $\square$

Combined with the definition of the  $\mathcal{I}$ -intersection closure, we obtain

**Corollary 3.4.** *The following statements hold:*

- (i) *If  $\Sigma$  is a circular split system for some circular ordering of  $X$  then  $\mathcal{I}(\Sigma)$  is also circular for that ordering.*
- (ii) *If  $N$  is a 1-nested network on  $X$  then  $\Sigma(N)$  is  $\mathcal{I}$ -intersection closed. Furthermore,  $N$  displays a split system  $\Sigma$  on  $X$  if and only if  $N$  displays  $\mathcal{I}(\Sigma)$ .*

The next observation is almost trivial and is used in the proof of Theorem 3.6.

**Lemma 3.5.** *Suppose  $x \in X$  and  $S_1, S_2$ , and  $S_3$  are three distinct splits of  $X$  such that  $S_3(x) \subseteq S_1(x)$ ,  $S_3$  and  $S_2$  are compatible and  $S_1$  and  $S_2$  are incompatible. Then  $S_3(x) \subseteq S_2(x)$  or  $S_2(x) \subseteq S_3(x)$ .*

*Proof.* Since  $S_2$  and  $S_3$  are compatible either  $S_2(x) \subseteq S_3(x)$  or  $S_3(x) \subseteq S_2(x)$  or  $\overline{S_3(x)} \subseteq \overline{S_2(x)}$  must hold. If  $\overline{S_3(x)} \subseteq \overline{S_2(x)}$  held then  $\emptyset \neq \overline{S_1(x)} \cap \overline{S_2(x)} \subseteq \overline{S_3(x)} \cap \overline{S_2(x)} = S_2(x) \cap \overline{S_2(x)} = \emptyset$  follows which is impossible.  $\square$

For clarity of presentation we remark that for the proof of Theorem 3.6, we will assume that if a given split  $S$  of a 1-nested network  $N$  has multiplicity at least two in  $\Sigma(N)$  then  $S$  is displayed by a cycle  $C$  of  $N$  (rather than by a cut-edge of  $N$ ). Furthermore, we denote the split system of  $X$  induced by a cycle  $C$  of a 1-nested network  $N$  on  $X$  by  $\Sigma(C)$ . Clearly,  $\Sigma(C) \subseteq \Sigma(N)$  holds.

**Theorem 3.6.** *Suppose  $\Sigma$  is a split system on  $X$  that contains all trivial splits of  $X$ . Then the following hold:*

- (i) *There exists a 1-nested network  $N$  on  $X$  such that  $\Sigma = \Sigma(N)$  if and only if  $\Sigma$  is circular and  $\mathcal{I}$ -intersection closed.*
- (ii) *A maximal partially-resolved 1-nested network  $N$  is a level-1 network if and only if there exists no split of  $X$  not contained in  $\Sigma(N)$  that is compatible with every split in  $\Sigma(N)$ .*

*Proof.* (i): Assume first that there exists a 1-nested network  $N$  on  $X$  such that  $\Sigma = \Sigma(N)$ . Then arguments similar to the ones used in [17, Theorem 2] to establish that the split system induced by a level-1 network is circular imply that  $\Sigma(N)$  is circular. Hence,  $\Sigma$  must be circular. That  $\Sigma$  is  $\mathcal{I}$ -intersection closed follows by Corollary 3.4(ii).

Conversely, assume that  $\Sigma$  is circular and  $\mathcal{I}$ -intersection closed. Then there clearly exists a 1-nested network  $N$  such that  $\Sigma \subseteq \Sigma(N)$ . Let  $N$  be such a network such that  $|\Sigma(N)|$  is minimal among all 1-nested networks on  $X$  satisfying this set inclusion. Without loss of generality, we may assume that  $N$  is maximal partially-resolved. We show that, in fact,  $\Sigma = \Sigma(N)$  holds. Assume for contradiction that this is not the case, that is, there exists a split  $S_0 \in \Sigma(N) - \Sigma$ . Since, by definition of a phylogenetic network,  $\Sigma(N)$  contains all trivial splits of  $X$  it follows that  $S_0$  cannot be a trivial split of  $X$ . Also and in view of the remark preceding the statement of the theorem,  $S_0$  is induced by either (a) deleting a cut-edge  $e = \{u, v\}$  of  $N$  and neither  $u$  nor  $v$  are contained in a cycle of  $N$  or (b) deleting two distinct edges of the same cycle of  $N$ .

Assume first that Case (a) holds. Then collapsing  $e$  results in a 1-nested network  $N'$  on  $X$  for which  $\Sigma \subseteq \Sigma(N')$  holds. But then  $|\Sigma(N')| < |\Sigma(N)|$  which is impossible in view of the choice of  $N$ . Thus, Case (b) must hold, that is,  $S_0$  is induced by deleting two distinct edges  $e = \{u, v\}$  and  $e' = \{u', v'\}$  of the same cycle  $C$  of  $N$ . Let  $x$  and  $y$  be two elements of  $X$  for which there exists a path from  $u$  and  $v$ , respectively, which does not cross an edge of  $C$ . Consider the sets  $\Sigma_x := \{S \in \Sigma \cap \Sigma(C) : S(x) \subseteq S_0(x)\}$ , and  $\Sigma_y := \{S \in \Sigma \cap \Sigma(C) : S(y) \subseteq S_0(y)\}$ . If  $\Sigma_x$  is non empty then choose some  $S_x \in \Sigma_x$  such that  $|S_x(x)|$  is maximal among the splits contained in  $\Sigma_x$ . Similarly, define the split  $S_y$  for  $\Sigma_y$  if  $\Sigma_y$  is non-empty. Otherwise let  $S_x$  be the m-split of  $C$  such that  $S_x(x) \subseteq S_0(x)$ . Similarly, let  $S_y$  be the m-split of  $C$  such that  $S_y(y) \subseteq S_0(y)$  in case  $\Sigma_y$  is empty. Then Corollary 3.4(ii) implies that the split

$$S^* = S_x(x) \cup S_y(y) | \overline{S_x(x)} \cap \overline{S_y(y)}$$

is contained in  $\Sigma(N)$  (see Figure 4(i) for an illustration).

We next show that  $S^*$  is compatible with every split in  $\Sigma$ . To this end we first claim that every split  $S' \in \Sigma$  that is incompatible with  $S^*$  must be compatible with at least one of  $S_x$  and  $S_y$ . To see this, let  $S' \in \Sigma$  such that  $S'$  and  $S^*$  are incompatible. Then  $S'$  must be displayed by  $C$ . For contradiction, assume that  $S'$  is incompatible with both of  $S_x$  and  $S_y$ . Let  $z \in X$  such that  $S^*(x) \neq S^*(z)$  and let  $u'' \in V(C)$  such that  $S_x(x)$  is the interval  $[u, u'']$ . Choose some element  $x'' \in X$  such that there exists a path from  $x''$  to  $u''$  that does not cross an edge contained in  $C$ . Similarly, let  $v'' \in V(C)$  such that  $S_y(y)$  is the interval  $[v'', v]$ .

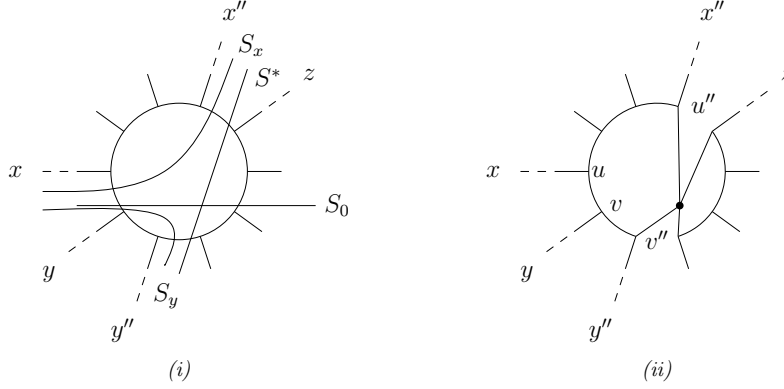


Figure 4: (i) An illustration of the reduction process considered in the proof of Case (a) of Theorem 3.6. (ii) Again for that theorem, the graph  $G'$  obtained from  $N$  by adding subdivision vertices  $r$  and  $r'$ .

Choose some element  $y'' \in X$  such that there exists a path from  $y'$  to  $v''$  that does not cross an edge contained in  $C$ . Then since  $S'$  is incompatible with  $S_x$  and  $S_y$  and displayed by  $C$  it follows that  $S'(x'') = S'(y'') = S'(z)$ . Hence,  $S^*(z) \subseteq S'(z)$ . But then  $S^*$  and  $S'$  are not incompatible which is impossible. Thus  $S'$  cannot be incompatible with both of  $S_x$  and  $S_y$ , as claimed.

To see that  $S^*$  is compatible with every split in  $\Sigma$ , we may, in view of the above claim, assume without loss of generality that  $S'$  is compatible with  $S_x$ . Then Lemma 3.5 applied to  $S'$ ,  $S^*$ , and  $S_x$  implies  $S_x(x) \subsetneq S'(x)$  or  $S'(x) \subsetneq S_x(x)$ . If  $S'(x) \subsetneq S_x(x)$  held then  $\emptyset \neq S'(x) \cap \overline{S^*(x)} \subseteq S_x(x) \cap \overline{S^*(x)} = \emptyset$  follows which is impossible. Hence,  $S_x(x) \subsetneq S'(x)$ . We distinguish between the cases that (α)  $S_y$  and  $S'$  are compatible and (β) that they are incompatible.

Case (α): Since  $S_y$  and  $S'$  are compatible, similar arguments as above imply that  $S_y(y) \subsetneq S'(y)$ . Then the definition of  $S^*$  combined with the assumption that  $S'$  and  $S^*$  are incompatible implies that  $S'(x) \neq S'(y)$ . But then  $S'$  and  $S_0$  must be compatible, and so,  $S'(x) \subseteq S_0(x)$  or  $S_0(x) \subseteq S'(x)$  must hold. If  $S'(x) \subseteq S_0(x)$  held then  $S' \in \Sigma_x$  which is impossible in view of the choice of  $S_x$  as  $S_x(x) \subsetneq S'(x)$ . Thus,  $S_0(x) \subseteq S'(x)$  must hold. But then  $S_y(y) \subsetneq S'(y) \subseteq S_0(y)$  and so  $S' \in \Sigma_y$  which is impossible in view of the choice of  $S_y$ . Thus, Case (β) must hold.

Case (β): Since  $S_y$  and  $S'$  are incompatible the split

$$S'' = S'(x) \cap \overline{S_y(y)} | \overline{S'(x)} \cup S_y(y)$$

is contained in  $\Sigma$  because  $\Sigma$  is  $\mathcal{I}$ -intersection closed and clearly displayed by  $C$ . Note that  $x \in \overline{S''(y)}$  and so  $S''(x) = \overline{S''(y)}$  must hold. Moreover, since  $S'$  and  $S^*$  are incompatible we cannot have  $S''(x) = S_x(x)$  as  $S_x$  and  $S^*$  are compatible. But then  $S_0$  and  $S''$  cannot be compatible. Indeed, if  $S_0$  and  $S''$  were compatible then since  $y \in S_0(y) \cap S''(y)$ ,  $x \in \overline{S_0(y)} \cap \overline{S''(y)}$ , and, because of  $S_x(x) \subsetneq S'(x)$ , also  $\overline{S_0(y)} \cap S''(y) = S_0(x) \cap S''(y) = S_0(x) \cap (\overline{S'(x)} \cup S_y(y)) \subseteq$

$S_0(x) \cap \overline{S_x(x)} \neq \emptyset$  holds, it follows that  $\overline{S''(y)} \subseteq \overline{S_0(y)}$ , as required. Hence,  $S''(x) = S''(y) \subseteq \overline{S_0(y)} = S_0(x)$  and so  $S'' \in \Sigma_x$  which is impossible in view of the choice of  $S_x$  as  $S_x(x) \neq S''(x)$  and  $S_0(x) \neq S''(x)$ . Thus,  $S_0$  and  $S''$  must be incompatible. But this is also impossible since the interval on  $C$  corresponding to  $S''(x)$  contains the interval  $[x, z]$  which induces the split  $S_0$  and so  $S_0$  and  $S''$  must be compatible. This final contradiction completes that proof that  $S^*$  is compatible for every split in  $\Sigma$ .

To conclude, let  $G$  be a new graph obtained from  $N$  by adding a subdivision vertex  $r$  and  $r'$ , respectively, to each of two edges whose deletion induces the split  $S^*$  (see Figure 4(ii) for an illustration). Then, the graph  $G'$  obtained from  $G$  by identifying  $r$  and  $r'$  is again a 1-nested network on  $X$ . By construction,  $S_0 \in \hat{\Sigma} := \{S \in \Sigma(N) : S \text{ is incompatible with } S^*\}$  clearly holds and so  $\Sigma(G') = \Sigma(N) - \hat{\Sigma} \subsetneq \Sigma(N)$ . Since, by the above, every split in  $\Sigma$  is compatible with  $S^*$  it follows that  $\Sigma \subseteq \Sigma(G')$ . But this is impossible in view of the choice of  $N$ . Hence, the split  $S_0$  cannot exist and, thus,  $\Sigma = \Sigma(N)$ .

(ii) Suppose  $N$  is a maximal partially-resolved 1-nested network. Assume first that  $N$  is a level-1 network on  $X$  and, for contradiction, that there exists some split  $S$  of  $X$  not contained in  $\Sigma(N)$  that is compatible with every split in  $\Sigma(N)$ . Then  $S$  cannot be a trivial split of  $X$ . Let  $N'$  be the graph obtained from  $N$  by deleting from each cycle of  $N$  one of its edges and suppressing resulting degree two vertices. Clearly  $N'$  is a phylogenetic tree on  $X$  and since every non-leaf vertex of  $N$  had degree three every such vertex in  $N'$  must also have degree three. Hence,  $\Sigma(N')$  is a maximal compatible split system on  $X$ . Since  $S$  is compatible with every split of  $\Sigma(N)$  and  $\Sigma(N') \subseteq \Sigma(N)$  it follows that  $\Sigma(N') \cup \{S\}$  is also compatible which is impossible in view of the maximality of  $\Sigma(N')$ .

Conversely, assume that there exists no split of  $X$  not contained in  $\Sigma(N)$  that is compatible with every split in  $\Sigma(N)$ . Then if  $N$  is not level-1 it contains a vertex  $v$  of degree  $k \geq 4$ , that does not belong to a cycle of  $N$ . Let  $X_1, \dots, X_k$  be the partition of  $X$  obtained by deletion of  $v$  (suppressing incident edges). Then there exist  $i, j \in \{1, \dots, k\}$  distinct, say  $i = 1$  and  $j = 2$ , such that the split  $S := X_1 \cup X_2 | \bigcup_{i=3}^k X_i$  is compatible with every split in  $N$ . Since  $S$  does not belong to  $\Sigma(N)$  this is impossible.  $\square$

Note that Theorem 3.6 allows one to decide if for a split system  $\Sigma$  of  $X$  there exists a 1-nested network  $N$  on  $X$  such that  $\Sigma = \Sigma(N)$ . However it does not provide a tool for how to construct such a network. The provision of such a tool is the purpose of the next two sections.

#### 4. Optimality and the analogue of the Split Equivalence Theorem

In this section, we turn our attention towards constructing 1-nested networks from circular split systems. In particular, we show that for any circular split system  $\Sigma$  on  $X$  it is possible to construct a, in a well-defined sense, optimal 1-nested network on  $X$  in  $\mathcal{O}(|X|^2 + |\Sigma|^2)$  time (Theorem 4.7). Central to our proof is Theorem 4.5 in which we characterize circular split systems whose

$\mathcal{I}$ -intersection closure is (set-inclusion) maximal in terms of their so called incompatibility graphs. As a consequence, we obtain the analog of the “Splits-Equivalence Theorem” (see Section 1) for 1-nested networks (Corollary 4.8). For phylogenetic trees this theorem is fundamental and characterizes split systems  $\Sigma$  for which there exists a, up to isomorphism, unique phylogenetic tree  $T$  for which  $\Sigma = \Sigma(T)$  holds.

We start with introducing some more terminology. Suppose  $\Sigma$  is a circular split system on  $X$ . Then we say that  $\Sigma$  is *maximal circular* if for all split system  $\Sigma'$  that contain  $\Sigma$ , we have  $\Sigma = \Sigma'$ . As the next result illustrates, maximal circular split systems of  $X$  and 1-nested networks on  $X$  are closely related.

**Lemma 4.1.** *A split system  $\Sigma$  on  $X$  is maximal circular if and only if there exists a simple level-1 network  $N$  on  $X$  such that  $\Sigma = \Sigma(N)$ .*

*Proof.* Let  $\Sigma$  be a split system on  $X$ . Assume first that  $\Sigma$  is maximal circular. Then, exists a simple level-1 network  $N$  on  $X$  such that  $\Sigma \subseteq \Sigma(N)$ . Since  $\Sigma(N)$  is clearly a circular split system on  $X$  the maximality of  $\Sigma$  implies  $\Sigma = \Sigma(N)$ .

Conversely, assume that  $N$  is a simple level-1 network such that  $\Sigma = \Sigma(N)$ . Then since  $\Sigma(N)$  is a circular split system on  $X$  so is  $\Sigma$ . Assume for contradiction that  $\Sigma$  is not maximal circular, that is, there exists a split  $S = A|\bar{A} \in \Sigma$  that is not contained in  $\Sigma(N)$ . Then  $A$  and  $\bar{A}$  are both intervals on the circular ordering of  $X$  induced by  $\Sigma(N)$ . Hence,  $S$  is induced by a minimal cut of  $N$  and, so,  $S \in \Sigma(N)$  which is impossible.  $\square$

Note that since a maximal circular split system on  $X$  must necessarily contain all 2-splits of  $X$  obtainable as a minimal cuts in the associated simple level-1 network on  $X$ , it follows that that ordering of  $X$  is unique. The next result suggests that systems of such splits suffice to generate a maximal circular split system. To state it, suppose  $x_1, \dots, x_{n-1}, x_n, x_{n+1} = x_1$  is a circular ordering of  $X$  and put  $\Sigma_d := \{\{x_i, x_{i+1}\} | X - \{x_i, x_{i+1}\} : 1 \leq i \leq n\}$ . Clearly,  $\Sigma_d$  is a circular split system on  $X$ .

In view of Lemma 4.1, we say that a circular ordering *displays* a split system  $\Sigma$  if  $\Sigma$  is displayed by the simple level-1 network associated to  $\Sigma$ .

**Lemma 4.2.** *Suppose  $\sigma : x_1, \dots, x_{n-1}, x_n, x_{n+1} = x_1$  is a circular ordering of  $X$ . Then  $\mathcal{I}(\Sigma_d)$  is a maximal circular split system on  $X$ .*

*Proof.* Since the result is trivial for  $n = 3$ , we may assume without loss of generality that  $n \geq 4$ . We proceed by induction on the size  $1 \leq l \leq \frac{n}{2}$  of a split  $S$  displayed by  $\sigma$ . Suppose first that  $l = 1$ . Then there exists some  $i \in \{1, \dots, n\}$  such that  $S = x_i | X - \{x_i\}$ . Clearly,  $S_1 = \{x_i, x_{i-1}\} | X - \{x_i, x_{i-1}\}$  and  $S_2 = \{x_i, x_{i+1}\} | X - \{x_i, x_{i+1}\}$  are contained in  $\Sigma_d$  and incompatible. Hence,  $S = S_1(x_i) \cap S_2(x_i) | X - (S_1(x_i) \cap S_2(x_i)) \in \iota(S_1, S_2) \subseteq \mathcal{I}(\Sigma_d)$ .

Now assume that  $l \geq 2$  and that all splits of  $X$  displayed by  $\sigma$  of size at most  $l - 1$  are contained in  $\mathcal{I}(\Sigma_d)$ . Since  $S$  is displayed by  $\sigma$  there exists some  $i \in \{1, \dots, n\}$  such that  $S = [x_i, x_{i+l-1}] | X - [x_i, x_{i+l-1}]$ . Without loss of generality we may assume that  $i = 1$ . Then  $S = [x_1, x_l] | X - [x_1, x_l]$ . Consider

the splits  $S_1 = [x_1, x_{l-1}]|X - [x_1, x_{l-1}]$  and  $S_2 = \{x_{l-1}, x_l\}|X - \{x_{l-1}, x_l\}$  displayed by  $\sigma$ . By induction,  $S_1, S_2 \in \mathcal{I}(\Sigma_d)$  since the size of  $S_2$  is two and that of  $S_1$  is at most  $l - 1$ . Furthermore,  $S_1$  and  $S_2$  are incompatible. Since  $S = S_1(x_{l-1}) \cup S_2(x_{l-1})|X - (S_1(x_{l-1}) \cup S_2(x_{l-1})) \in \iota(S_1, S_2) \subseteq \mathcal{I}(\Sigma_d)$ , the lemma follows.  $\square$

We next employ Lemma 4.2 to obtain a sufficient condition on a circular split system  $\Sigma$  for  $\mathcal{I}(\Sigma)$  to be maximal circular. Central to this is the concept of the *incompatibility graph*  $Incomp(\Sigma)$  of a split system  $\Sigma$ . For  $\Sigma$  a split system on  $X$  the vertex set of that graph is  $\Sigma$  and any two distinct splits of  $\Sigma$  are joined by an edge in  $Incomp(\Sigma)$  if they are incompatible. We denote the set of connected components of  $Incomp(\Sigma)$  by  $\pi_0(\Sigma)$  and, by abuse of terminology, refer to the vertex set of an element in  $\pi_0(\Sigma)$  as a *connected component of  $Incomp(\Sigma)$* . For example,  $Incomp(\Sigma_d)$  is a cycle of length  $|\Sigma_d|$  whenever  $n \geq 5$ . Furthermore,  $\Sigma$  is compatible if and only if  $|\Sigma_0| = 1$  holds for all  $\Sigma_0 \in \pi_0(\Sigma)$ .

We next clarify the relationship between the incompatibility graph and  $\mathcal{I}$ -intersection closure of a split system.

**Lemma 4.3.** *Suppose  $\Sigma$  is a split system on  $X$ . Then there cannot exist two distinct connected components  $\Sigma_1, \Sigma_2 \in \pi_0(\Sigma)$  and splits  $S_1 \in \mathcal{I}(\Sigma_1)$  and  $S_2 \in \mathcal{I}(\Sigma_2)$  such that  $S_1$  and  $S_2$  are incompatible.*

*Proof.* Assume for contradiction that there exist two connected components  $\Sigma_1, \Sigma_2 \in \pi_0(\Sigma)$  and splits  $S_1 \in \mathcal{I}(\Sigma_1)$  and  $S_2 \in \mathcal{I}(\Sigma_2)$  such that  $S_1$  and  $S_2$  are incompatible. Then  $S_1 \in \Sigma_1$  and  $S_2 \in \Sigma_2$  cannot both hold as otherwise  $\Sigma_1 = \Sigma_2$ . Assume without loss of generality that  $S_1 \notin \Sigma_1$ . Let  $\Sigma^0 := \Sigma_1 \subsetneq \Sigma^1 \subsetneq \dots \subsetneq \Sigma^k := \mathcal{I}(\Sigma_1)$ ,  $k \geq 1$  be a finite sequence such that, for all  $1 \leq i \leq k$ , a split in  $\Sigma^i$  either belongs to  $\Sigma^{i-1}$  or is an  $\mathcal{I}$ -intersection between two splits  $S, S' \in \Sigma^{i-1}$  and  $\iota(S, S') \not\subseteq \Sigma^{i-1}$ . Then, there exists some  $i^* > 0$  such that  $S_1 \in \Sigma^{i^*} - \Sigma^{i^*-1}$ . After possibly renaming  $S_1$ , we may assume without loss of generality, that  $i^*$  is such that for all  $1 \leq i \leq i^* - 1$  there exists no split in  $\Sigma^i$  that is incompatible with  $S_2$ . Hence, there must exist two splits  $S$  and  $S'$  in  $\Sigma^{i^*-1}$  distinct such that  $S_1 \in \iota(S, S')$ . Since  $S_2$  and  $S_1$  are incompatible, it follows that  $S_2$  is incompatible with one of  $S$  and  $S'$ , which is impossible by the choice of  $i^*$ .  $\square$

Armed with this result, we next relate for a split system  $\Sigma$  the sets  $\pi_0(\mathcal{I}(\Sigma))$  and  $\pi_0(\Sigma)$ .

**Lemma 4.4.** *Suppose  $\Sigma$  is a split system on  $X$ . Then the following hold*

- (i)  $\mathcal{I}(\Sigma) = \bigcup_{\Sigma_0 \in \pi_0(\Sigma)} \mathcal{I}(\Sigma_0)$ .
- (ii)  $\pi_0(\mathcal{I}(\Sigma_0)) \subseteq \pi_0(\mathcal{I}(\Sigma))$ , for all  $\Sigma_0 \in \pi_0(\Sigma)$ . In particular,  $\pi_0(\mathcal{I}(\Sigma)) = \bigcup_{\Sigma_0 \in \pi_0(\Sigma)} \pi_0(\mathcal{I}(\Sigma_0))$ .

*Proof.* (i) Let  $\Sigma_0 \in \pi_0(\Sigma)$  and put  $\mathcal{A} := \bigcup_{\Sigma' \in \pi_0(\Sigma)} \mathcal{I}(\Sigma')$ . Note that since  $\Sigma = \bigcup_{\Sigma' \in \pi_0(\Sigma)} \Sigma'$ , we trivially have  $\Sigma \subseteq \mathcal{A} \subseteq \mathcal{I}(\Sigma)$ . To see that  $\mathcal{I}(\Sigma) \subseteq \mathcal{A}$

note that Lemma 4.3 implies that any two incompatible splits in  $\mathcal{A}$  must be contained in the same connected component so must be their  $\mathcal{I}$ -intersection. Thus,  $\mathcal{A}$  is  $\mathcal{I}$ -intersection closed. Since  $\Sigma \subseteq \mathcal{A}$  we also have  $\mathcal{I}(\Sigma) \subseteq \mathcal{I}(\mathcal{A}) = \mathcal{A}$  and, so,  $\mathcal{A} = \mathcal{I}(\Sigma)$  follows.

(ii) Suppose  $\Sigma_0 \in \pi_0(\Sigma)$  and let  $\bar{\Sigma}_0 \in \pi_0(\mathcal{I}(\Sigma_0))$ . To establish that  $\bar{\Sigma}_0 \in \pi_0(\mathcal{I}(\Sigma))$  note that since  $\bar{\Sigma}_0$  is connected in  $\mathcal{I}(\Sigma_0)$  it also is connected in  $\mathcal{I}(\Sigma)$ . Hence, it suffices to show that every split in  $\bar{\Sigma}_0$  is compatible with every split in  $\mathcal{I}(\Sigma) - \bar{\Sigma}_0$ . Suppose  $S_1 \in \bar{\Sigma}_0$  and  $S_2 \in \mathcal{I}(\Sigma) - \bar{\Sigma}_0 = (\mathcal{I}(\Sigma) - \mathcal{I}(\Sigma_0)) \cup (\mathcal{I}(\Sigma_0) - \bar{\Sigma}_0)$ . If  $S_2 \in \mathcal{I}(\Sigma_0) - \bar{\Sigma}_0$  then, by definition,  $S_1$  and  $S_2$  are compatible. So assume that  $S_2 \in \mathcal{I}(\Sigma) - \mathcal{I}(\Sigma_0)$ . Then Lemma 4.4(i) implies that  $S_2$  is compatible with every split in  $\mathcal{I}(\Sigma_0)$  and thus with  $S_1$  as  $\bar{\Sigma}_0 \subseteq \mathcal{I}(\Sigma_0)$ .  $\square$

To establish the next result which is central to Theorem 4.7, we require a further notation. Suppose  $\Sigma$  is a split system on  $X$ . Then we denote by  $\Sigma^-$  the split system obtained from  $\Sigma$  by deleting all trivial splits on  $X$ .

**Theorem 4.5.** *Let  $\Sigma$  be a circular split system on  $X$ . Then  $\mathcal{I}(\Sigma)$  is a maximal circular split system on  $X$  if and only if the following two conditions hold:*

- (i) *for all  $x, y \in X$  distinct, there exists some  $S \in \Sigma^-$  such that  $S(x) \neq S(y)$ ,*
- (ii)  *$\text{Incomp}(\Sigma^-)$  is connected.*

*Moreover, if (i) and (ii) hold then there exists an unique, up to isomorphism and partial-resolution, simple 1-nested network  $N$  on  $X$  such that  $\Sigma \subseteq \Sigma(N)$ .*

*Proof.* Let  $x_1, \dots, x_n, x_{n+1} = x_1$  denote an underlying circular ordering of  $X$  for  $\Sigma$ . Assume first that (i) and (ii) hold. We first show that  $\mathcal{I}(\Sigma^-)$  is maximal circular. To this end, it suffices to show that  $\Sigma_d \subseteq \mathcal{I}(\Sigma^-)$  since this implies that  $\mathcal{I}(\Sigma_d) \subseteq \mathcal{I}(\mathcal{I}(\Sigma^-)) \subseteq \mathcal{I}(\mathcal{I}(\Sigma)) = \mathcal{I}(\Sigma)$ . Combined with the fact that, in view of Lemma 4.2,  $\mathcal{I}(\Sigma_d)$  is maximal circular, it follows that  $\mathcal{I}(\Sigma_d) = \mathcal{I}(\Sigma^-) = \mathcal{I}(\Sigma)$ . Hence,  $\mathcal{I}(\Sigma)$  is maximal circular.

Assume for contradiction that there exists some  $i \in \{1, \dots, n\}$  such that the split  $S^* = x_i x_{i+1} | x_{i+2}, \dots, x_{i-1}$  of  $\Sigma_2$  is not contained in  $\mathcal{I}(\Sigma)$ . Then, by assumption, there exist two splits  $S$  and  $S'$  in  $\Sigma$  such that  $S(x_i) \neq S(x_{i-1})$  and  $S'(x_{i+1}) \neq S'(x_{i+2})$ . Let  $P_{SS'}$  denote a shortest path in  $\text{Incomp}(\Sigma)$  joining  $S$  and  $S'$ . Without loss of generality, let  $S$  and  $S'$  be such that the path  $P_{SS'}$  is as short as possible. Let  $S_0 = S, S_1, \dots, S_k = S'$  denote that path. The next lemma is central to the proof

**Lemma 4.6.** *For all  $0 \leq j \leq k$ , we have  $S_j(x_i) = S_j(x_{i+1})$ .*

*Proof.* First observe that  $S_j(x_i) = S_j(x_{i-1})$  and  $S_j(x_{i+1}) = S_j(x_{i+2})$  must hold for all  $0 < j < k$ . Indeed, if there existed some  $j \in \{1, \dots, k-1\}$  such that  $S_j(x_i) \neq S_j(x_{i-1})$  then the path  $S_j, S_{j+1}, \dots, S_k$  would be shorter than  $P_{SS'}$  in contradiction to the choice of  $S$  and  $S'$ . Similar arguments also imply that  $S_j(x_{i+1}) = S_j(x_{i+2})$  holds for all  $j \in \{1, \dots, k-1\}$ .

Assume for contradiction that there exists  $0 \leq j \leq k$  such that  $S_j(x_i) \neq S_j(x_{i+1})$ . Without loss of generality, we may assume that for all  $0 \leq l \leq j-1$  we have that  $S_l(x_i) = S_l(x_{i+1})$ . Then since a trivial split cannot be incompatible with any other split on  $X$  we cannot have  $j \in \{0, k\}$ . Thus, the

splits  $S_{j-1}$  and  $S_{j+1}$  must exist. Note that they cannot be incompatible, since otherwise the path from  $S$  to  $S'$  obtained by deleting  $S_j$  from  $P_{SS'}$  is shorter than  $P_{SS'}$  which is impossible. So  $S_{j-1}$  and  $S_{j+1}$  must be compatible. Clearly,  $x_i \in S_{j+1}(x_i) \cap S_{j-1}(x_i)$ . We next establish that  $\overline{S_{j+1}(x_i)} \cap \overline{S_{j-1}(x_i)} = \emptyset$  cannot hold implying that either  $S_{j+1}(x_i) \cap \overline{S_{j-1}(x_i)} = \emptyset$  or  $\overline{S_{j+1}(x_i)} \cap S_{j-1}(x_i) = \emptyset$ .

Indeed, let  $q \in \{1, \dots, n\}$  such that  $S_j = x_{i+1} \dots x_q | x_{q+1} \dots x_i$ . We claim that  $x_q \in \overline{S_{j+1}(x_i)} \cap \overline{S_{j+1}(x_i)}$ . Assume by contradiction that  $x_q \in S_{j-1}(x_i)$ . Then  $S_{j-1}(x_i)$  is an interval of  $X$  containing  $\{x_i, x_q\}$  and, so, either  $S_{j-1}(x_i) \supseteq [x_i, x_q] \supset S_j(x_{i+1})$  or  $S_{j-1}(x_i) \supseteq [x_q, x_i] \supset S_j(x_i)$ . But both are impossible in view of the fact that  $S_{j-1}$  and  $S_j$  are incompatible.

Now assume that  $S_{j+1}(x_i) \cap \overline{S_{j-1}(x_i)} = \emptyset$ , that is,  $S_{j+1}(x_i) \subseteq S_{j-1}(x_i)$ . We postulate that then  $S_{j+1}(x_i) \subseteq S_0(x_i)$  must hold which is impossible since  $x_{i-1} \in S_{j+1}(x_i)$  and  $S_0(x_i) \neq S_0(x_{i-1})$ . Indeed, the choice of  $S$  and  $S'$  implies that  $S_{j+1}$  and  $S_l$  must be compatible, for all  $0 \leq l \leq j-2$ . By Lemma 3.5 applied to  $S_{j-1}$ ,  $S_{j-2}$ , and  $S_{j+1}$  it follows that  $S_{j+1}(x_i) \subseteq S_{j-2}(x_i)$  or  $S_{j-2}(x_i) \subseteq S_{j+1}(x_i)$ . In the latter case we obtain  $S_{j-2}(x_i) \subseteq S_{j-1}(x_i)$  which is impossible since  $S_{j-1}$  and  $S_{j-2}$  are incompatible. Thus,  $S_{j+1}(x_i) \subseteq S_{j-2}(x_i)$ . Repeated application of this argument implies that, for all  $0 \leq l \leq j-2$  we have  $S_{j+1}(x_i) \subseteq S_l(x_i)$ , as required.

Finally, assume that  $S_{j-1}(x_i) \cap \overline{S_{j+1}(x_i)} = \emptyset$ , that is,  $S_{j-1}(x_i) \subseteq S_{j+1}(x_i)$ . Then similar arguments as in the previous case imply that  $S_{j-1}(x_i) \subseteq S_k(x_i)$ . But this is impossible since  $x_{i+1}, x_{i+2} \in S_{j-1}(x_i)$  and  $S_k(x_i) = S_k(x_{i+1}) \neq S_k(x_{i+2})$ . Thus,  $S_j(x_i) = S_j(x_{i+1})$  must hold for all  $0 \leq j \leq k$  which concludes the proof of Lemma 4.6.  $\square$

Continuing with the proof of Theorem 4.5, we claim that the splits

$$T_j := T_{j-1}(x_i) \cap S_j(x_i) | \overline{T_{j-1}(x_i)} \cup \overline{S_j(x_i)}$$

where  $j \in \{1, \dots, k\}$  and  $T_0 := S_0$  are contained in  $\mathcal{I}(\Sigma)$ . Assume for contradiction that there exists some  $j \in \{0, \dots, k\}$  such that  $T_j \notin \mathcal{I}(\Sigma)$ . Then  $j \neq 0$  because  $S \in \mathcal{I}(\Sigma)$ , and  $j \neq 1$  since  $T_1 \in \iota(S, S_1)$  and  $S, S_1 \in \Sigma$ . Without loss of generality, we may assume that  $j$  is such that for all  $1 \leq l \leq j-1$  we have that  $T_l \in \mathcal{I}(\Sigma)$ . Then  $T_{j-1}$  and  $S_j$  cannot be incompatible and so  $T_{j-1}(x_i) \subseteq S_j(x_i)$ , or  $S_j(x_i) \subseteq T_{j-1}(x_i)$ , or  $\overline{S_j(x_i)} \subseteq \overline{T_{j-1}(x_i)}$  must hold. But  $S_j(x_i) \subseteq T_{j-1}(x_i)$  cannot hold since then  $\overline{S_{j-1}(x_i)} \subseteq \overline{T_{j-2}(x_i)} \cup \overline{S_{j-1}(x_i)} = \overline{T_{j-1}(x_i)} \subseteq \overline{S_j(x_i)}$  which is impossible as  $S_{j-1}$  and  $S_j$  are incompatible. Also,  $\overline{S_j(x_i)} \subseteq \overline{T_{j-1}(x_i)}$  cannot hold since then  $\overline{S_j(x_i)} \subseteq T_{j-1}(x_i) = T_{j-2}(x_i) \cap S_{j-1}(x_i) \subseteq S_{j-1}(x_i)$  which is again impossible as  $S_{j-1}$  and  $S_j$  are incompatible. Thus,  $T_{j-1}(x_i) \subseteq S_j(x_i)$  and so  $T_j(x_i) = T_{j-1}(x_i)$ . Consequently,  $T_j = T_{j-1} \in \mathcal{I}(\Sigma)$  which is also impossible and therefore proves the claim. Thus,  $T_j \in \mathcal{I}(\Sigma)$ , for all  $0 \leq j \leq k$ . Combined with Lemma 4.6 it follows that, for all  $0 \leq j \leq k$ , we also have  $T_j(x_i) = T_j(x_{i+1})$ . Consequently,  $\{x_i, x_{i+1}\} \subseteq T_k(x_i)$ . Combined with the facts that  $T_k(x_i)$  is an interval on  $X$  and  $x_{i-1} \notin S_0(x_i)$ , and similarly,  $x_{i+2} \notin S_k(x_i)$  it follows that  $\{x_i, x_{i+1}\} = T_k(x_i)$ . Hence,  $S^* = T_k \in \mathcal{I}(\Sigma)$ , which is impossible. Thus,  $\Sigma_d \subseteq \mathcal{I}(\Sigma^-)$  and so  $\mathcal{I}(\Sigma_d) = \mathcal{I}(\Sigma^-)$ .



Conversely, assume that  $\mathcal{I}(\Sigma)$  is maximal circular. Then  $\mathcal{I}(\Sigma)$  clearly satisfies Properties (i) and (ii) that is, for all  $x, y \in X$  distinct there exists some  $S \in \mathcal{I}(\Sigma)^-$  such that  $S(x) \neq S(y)$  and  $\text{Incomp}(\mathcal{I}(\Sigma)^-)$  is connected. We need to show that  $\Sigma$  also satisfies Properties (i) and (ii). Assume for contradiction that  $\Sigma$  does not satisfy Property (i). Then there exist  $x, y \in X$  distinct such that for all splits  $S \in \Sigma^-$ , we have  $S(x) = S(y)$ . Let  $S \in \mathcal{I}(\Sigma)$  such that  $S(x) \neq S(y)$  and let  $S_1, S_2, \dots, S_l = S$  denote a sequence in  $\mathcal{I}(\Sigma)$  such that  $S_i \in \iota(S_{i-1}, S_{i-2})$ , for all  $3 \leq i \leq l$ . Without loss of generality we may assume that  $l$  is such that  $S_i(x) = S_i(y)$ , for all  $3 \leq i \leq l-1$ . Then  $S_j(x) = S_j(y)$ , for all  $j \in \{l-1, l-2\}$  and thus  $S(x) = S(y)$  which is impossible.

Next, assume for contradiction that  $\Sigma$  does not satisfy Property (ii). Let  $\Sigma_1$  and  $\Sigma_2$  denote two disjoint connected components of  $\text{Incomp}(\Sigma^-)$ . For  $i = 1, 2$ , let  $\bar{\Sigma}_i \in \pi_0(\mathcal{I}(\Sigma_i)^-)$  such that  $\Sigma_i \subseteq \bar{\Sigma}_i$ . Then,  $2 \leq |\Sigma_i| \leq |\bar{\Sigma}_i|$ , for all  $i = 1, 2$ . Combined with Lemma 4.4(ii), we obtain  $\bar{\Sigma}_1, \bar{\Sigma}_2 \in \pi_0(\mathcal{I}(\Sigma)^-)$ . Since  $\text{Incomp}(\mathcal{I}(\Sigma)^-)$  is connected, it follows for  $i = 1, 2$  that  $\bar{\Sigma}_i \subseteq \mathcal{I}(\Sigma_i)^- \subseteq \mathcal{I}(\Sigma)^- = \bar{\Sigma}_i$ . Thus,  $\mathcal{I}(\Sigma_1)^- = \mathcal{I}(\Sigma)^- = \mathcal{I}(\Sigma_2)^-$  and so the incompatibility graphs  $\text{Incomp}(\mathcal{I}(\Sigma_1)^-)$ ,  $\text{Incomp}(\mathcal{I}(\Sigma)^-)$  and  $\text{Incomp}(\mathcal{I}(\Sigma_2)^-)$  all coincide. Suppose  $S \in \Sigma_1$  and  $S' \in \Sigma_2$  and let  $P$  denote a shortest path in  $\text{Incomp}(\mathcal{I}(\Sigma)^-)$  joining  $S$  and  $S'$ . Then there must exist incompatible splits  $S$  and  $S'$  in  $P$  such that  $S \in \Sigma_1 \subseteq \mathcal{I}(\Sigma_1)^- = \mathcal{I}(\Sigma)^- = \mathcal{I}(\Sigma_2)^-$  which is impossible in view of Lemma 4.3.

The remainder of the theorem follows from the facts that, by Lemma 4.2,  $\mathcal{I}(\Sigma)$  is maximal circular that, by Lemma 4.1, there exists a simple level-1 network  $N$  such that  $\mathcal{I}(\Sigma) = \Sigma(N)$ , that by Corollary 3.4(ii), a 1-nested network displays  $\mathcal{I}(\Sigma)$  if and only if it displays  $\Sigma$ , and that the split system  $\Sigma_d$  uniquely determines the underlying circular ordering of  $X$ .  $\square$

Armed with this characterization, we are now ready to establish Theorem 4.7

**Theorem 4.7.** *Given a circular split system  $\Sigma$  on  $X$ , it is possible to build, in time  $O(n^2 + |\Sigma|^2)$ , a 1-nested network  $N$  on  $X$  such that  $\Sigma \subseteq \Sigma(N)$  holds and  $|\Sigma(N)|$  is minimal. Furthermore,  $N$  is unique up to isomorphism and partial-resolution.*

*Proof.* Suppose  $\Sigma$  is a circular split system on  $X$ . Put  $\{V_1, \dots, V_l\} = \pi_0(\Sigma)$ . Without loss of generality we may assume that there exists some  $j \in \{1, \dots, l\}$  such that  $|V_i| = 1$  holds for all  $1 \leq i \leq j-1$  and  $|V_i| \geq 2$  for all  $j \leq i \leq l$ . Since  $\text{Incomp}(\Sigma)$  has  $l-j+1$  connected components with at least two vertices there exist  $l-j+1$  simple 1-nested networks  $N_i$  such that  $V_i \subseteq \Sigma(C_i)$  holds for the unique cycle  $C_i$  of  $N_i$ . By Theorem 4.5, it follows for all  $j \leq i \leq l$  that  $\Sigma(C_i) = \mathcal{I}(V_i)$  and that  $Q_i \subseteq \mathcal{I}(V_i)$ , where  $Q_i$  denotes the set of m-splits of  $C_i$ .

We claim that the split system  $\Sigma'$  on  $X$  given by

$$\Sigma' = \bigcup_{i=1}^{j-1} V_i \cup \bigcup_{i=j}^l Q_i \cup \bigcup_{x \in X} \{x|X-x\}$$

is compatible. Since  $\Sigma$  is circular there exists a 1-nested network  $N$  on  $X$  such that  $\Sigma \subseteq \Sigma(N)$ . Without loss of generality, we may assume that  $N$  is such

that  $|\Sigma(N)|$  is minimal among such networks. For clarity of exposition, we may furthermore assume that  $N$  is maximal partially-resolved. Then for all  $j \leq i \leq l$  there exists a cycle  $Z_i$  in  $N$  such that  $V_i \subseteq \Sigma(Z_i)$ . In fact,  $\mathcal{I}(V_i) = \Sigma(Z_i)$  must hold for all such  $i$ . Combined with the minimality of  $\Sigma(N)$ , it follows that there exists a one-to-one correspondence between the cycles of  $N$  and the set  $\mathcal{A} := \{\mathcal{I}(V_i) : j \leq i \leq l\}$  that maps a cycle  $Z$  of  $N$  to the split system  $\Sigma_C \in \mathcal{A}$  such that for some  $i^* \in \{j, \dots, l\}$  we have  $\Sigma_C = \mathcal{I}(V_{i^*})$  and  $V_{i^*} \subseteq \Sigma(Z)$ . Furthermore, for all  $1 \leq i \leq j - 1$  there exists a cut-edge  $e_i$  of  $N$  such that the split  $S_{e_i}$  induced on  $X$  by deleting  $e_i$  is the unique element in  $V_i$ .

Let  $T(N)$  denote the phylogenetic tree on  $X$  obtained from  $N$  by first shrinking every cycle  $Z$  of  $N$  to a vertex  $v_Z$  and then suppressing all resulting degree two vertices. Since this operation clearly preserves the splits in  $Q_i$ ,  $j \leq i \leq l$ , and also does not affect the cut-edges of  $N$  (in the sense that a cut edge of  $T(N)$  might correspond to a path in  $N$  of length at most 3 involving a cut-edge of  $N$  and one or two m-splits), it follows that  $\Sigma' = \Sigma(T(N))$ . Since any split system displayed by a phylogenetic tree is compatible the claim follows.

Since, in addition,  $\Sigma'$  also contains all trivial splits on  $X$ , it follows by the “Splits Equivalence Theorem” (see Section 1) that there exists a unique (up to isomorphism) phylogenetic tree  $T$  on  $X$  such  $\Sigma(T) = \Sigma'$ . Hence,  $T(N)$  and  $T$  must be isomorphic. But then reversing the aforementioned cycle-shrinking operation that gave rise to  $T(N)$  results in a 1-nested network  $N'$  on  $X$  such that  $\Sigma(N) = \Sigma(N')$ . Consequently,  $N'$  and  $N$  are isomorphic and so  $\Sigma \subseteq \Sigma(N')$ . Note that similar arguments also imply that  $N$  is unique up to partial-resolution and isomorphism.

To see the remainder of the theorem, note first that a maximal circular split system  $\Sigma$  on  $X$  has  $n(n - 1)/2$  splits. Thus, finding  $\text{Incomp}(\Sigma)$  can be accomplished in  $\mathcal{O}(|\Sigma|^2)$  time. Combined with the facts that  $X$  has at most  $n$  cycles and any binary unrooted phylogenetic tree on  $X$  has  $2n - 3$  cut-edges it follows that  $N'$  can be constructed in  $\mathcal{O}(n^2 + |\Sigma|^2)$  time.  $\square$

In consequence of Theorems 3.6 and 4.7, we obtain the 1-nested analogue of the “Splits Equivalence Theorem” (see Section 1).

**Corollary 4.8.** *Suppose  $\Sigma$  is a split system on  $X$  that contains all trivial splits of  $X$ . Then there exist a 1-nested network  $N$  on  $X$  such that  $\Sigma = \Sigma(N)$  if and only if  $\Sigma$  is circular and  $\mathcal{I}$ -intersection closed. Moreover, if such a network  $N$  exists then it is unique up to isomorphism and partial-resolution and can be constructed in  $\mathcal{O}(n^2 + |\Sigma|^2)$  time.*

As observed in Section 2, a 1-nested network also induces a multi-set of splits. This raises the question of an 1-nested analogue of the “Splits Equivalence Theorem” (see Section 1) for such collections. We will settle this question elsewhere.

## 5. Optimality and the Buneman graph

In this section, we investigate the interplay between the Buneman graph  $G(\Sigma)$  of a circular split system  $\Sigma$  and a 1-nested network displaying  $\Sigma$ . More

precisely, we first associate to a circular split system  $\Sigma$  a certain subgraph of  $G(\Sigma)$  which we obtain by replacing each block of  $G(\Sigma)$  by a structurally simpler graph which we call a marguerite. As it turns out, marguerites hold the key for constructing optimal 1-nested networks from circular split systems. We start with defining the Buneman graph and then review relevant properties.

Suppose  $\Sigma$  is a split system on  $X$  and let  $\mathcal{P}(X)$  denote the power set of  $X$ . Then the *Buneman graph*  $G(\Sigma)$  associated to  $\Sigma$  is the subgraph of the  $|\Sigma|$ -dimensional hypercube whose vertex set  $V(\Sigma) = V(G(\Sigma))$  is the set of all maps  $\phi : \Sigma \rightarrow \mathcal{P}(X)$  such that  $\phi(S) \in S$  holds for all  $S \in \Sigma$  and  $\phi(S) \cap \phi(S') \neq \emptyset$ , for all  $S, S' \in \Sigma$ . Note that  $V(\Sigma) \neq \emptyset$  since for all  $x \in X$  the *Kuratowski map* associated to  $x$  defined by putting  $\phi_x : \Sigma \rightarrow \mathcal{P}(X)$ :  $S \mapsto S(x)$  is contained in  $V(\Sigma)$ . The edge set  $E(\Sigma)$  comprises all sets  $\{\phi, \phi'\} \in \binom{V(\Sigma)}{2}$  such that the difference set  $\Delta(\phi, \phi') = \{S \in \Sigma : \phi(S) \neq \phi'(S)\}$  contains precisely one element. We say that a split  $S = A|B$  of  $X$  is *Bu-displayed* by  $G(\Sigma)$  if there exists a “ladder”  $E'$  of parallel edges whose deletion disconnects  $G(\Sigma)$  into two connected components one of whose vertex sets contains  $A$  and the other  $B$  (see e.g. [14, Lemma 4.5] for details where Bu-displayed is called displayed). Note that every split that is Bu-displayed by  $G(\Sigma)$  is also a minimal cut of  $G(\Sigma)$  and thus displayed by  $G(\Sigma)$ . However the converse need not hold.

To illustrate these definitions let  $X = \{1, \dots, 8\}$  and consider again the split system  $\Sigma$  displayed by the 1-nested network depicted in Fig. 2(i). Then the Buneman graph  $G(\Sigma)$  associated to  $\Sigma$  is depicted in Figure 1(ii).

### 5.1. Marguerites and Blocks

In this section, we first focus on the Buneman graph of a maximal circular split system and then introduce and study the novel concept of a marguerite. We start with collecting some relevant results.

For  $\Sigma$  a split system on  $X$ , the following five properties of  $G(\Sigma)$  are well-known (see e.g. [14, Chapter 4]).

- (Bi) The split system  $\Sigma(G(\Sigma))$  Bu-displayed by  $G(\Sigma)$  is  $\Sigma$ .
- (Bii) For  $\phi \in V(\Sigma)$  let  $\min(\phi(\Sigma))$  denote the set-inclusion minimal elements in  $\phi(\Sigma) := \{\phi(S) : S \in \Sigma\}$  and let  $\Sigma^{(\phi)}$  denote the set of pre-images of  $\min(\phi(\Sigma))$  under  $\phi$ . Then a vertex  $\psi \in V(\Sigma)$  is adjacent with  $\phi$  if and only if there exists some split  $S^* \in \Sigma^{(\phi)}$  such that  $\psi(S^*) = \overline{\phi(S^*)}$  and  $\psi(S) = \phi(S)$ , otherwise. In particular,  $|\Sigma^{(\phi)}|$  is the degree of  $\phi$  in  $G(\Sigma)$ .
- (Biii) In case  $\Sigma$  contains all trivial splits on  $X$  then  $\Sigma$  is compatible if and only if, when identifying each Kuratowski map  $\phi_x$  with its underlying element  $x \in X$ ,  $G(\Sigma)$  is a unrooted phylogenetic tree on  $X$  for which  $\Sigma(G(\Sigma)) = \Sigma$  holds. Moreover, and up to isomorphism,  $G(\Sigma)$  is unique.

Note that for any two distinct compatible splits  $S$  and  $S'$  of  $X$  there must exist a unique subset  $A \in S \cup S'$ , say  $A \in S$ , such that  $A \cap A' \neq \emptyset$  holds for all  $A' \in S'$ . Denoting that subset by  $\max(S|S')$ , we obtain

- (Biv) For  $\Sigma_1, \Sigma_2 \in \pi_0(\Sigma)$  distinct we have  $\max(S_1|S_2) = \max(S_1|S'_2)$ , for all  $S_1 \in \Sigma_1$  and all  $S_2, S'_2 \in \Sigma_2$ . In consequence,  $\max(S_1|\Sigma_2) := \max(S_1|S_2)$  is well-defined where  $S_1 \in \Sigma_1$  and  $S_2 \in \Sigma_2$  [14, Section 5].

A graph is called *2-connected* if, after deletion of any of its vertices, it remains connected or is an isolated vertex [16]. Calling a maximal 2-connected component of a graph  $G$  a *block* of  $G$  and denoting the set of blocks of  $G$  by  $\mathfrak{BI}(G)$  we obtain

- (Bv) The blocks of  $G(\Sigma)$  are in 1-1 correspondence with the connected components of  $Incomp(\Sigma)$ . More precisely the map  $\Theta : \pi_0(\Sigma) \rightarrow \mathfrak{BI}(G(\Sigma)) : \Sigma_0 \mapsto B(\Sigma_0) := \{\phi \in V(\Sigma) : \phi(S) = \max(S|\Sigma_0) \text{ holds for all } S \in \Sigma - \Sigma_0\}$  is a bijection [16, Theorem 5.1].

To illustrate these definitions, consider again the Buneman graph depicted in Figure 1(ii) and the splits  $S = 78|1 \dots 6$  and  $S' = 18|2 \dots 7$  both of which are Bu-displayed by that graph. Then for the marked vertex  $\phi$ , we have  $\phi(S) = \{7, 8\}$ . The block marked  $\mathcal{B}_1$  in that figure corresponds via  $\Theta$  to the connected component  $\Sigma_0 = \{S, S'\}$  and  $\max(S'|\Sigma_0) = X - \{2, 3, 4\}$ .

For the following assume that  $k \geq 4$  and that  $Y = \{X_1, \dots, X_k\}$  is a partition of  $X$ . For clarity of exposition, also assume that  $|X_i| = 1$  for all  $1 \leq i \leq k$  and that the unique element in  $X_i$  is denoted by  $i$ . Further, assume that  $\sigma$  is the lexicographical ordering of  $X$  where we put  $k+1 := 1$ . Let  $\Sigma_k$  denote the maximal circular split system displayed by  $\sigma$  bar the trivial splits of  $X$ . Since  $\Sigma_k$  contains all 2-splits displayed by  $\sigma$  it follows that  $|\pi_0(\Sigma_k)| = 1$  and, so,  $G(\Sigma_k)$  is a block in view of Property (Bv). To better understand the structure of  $B(\Sigma_k)$  consider for all  $1 \leq i \leq k$  and for all  $0 \leq j < k-3$  the map:

$$\phi_i^j : \Sigma_k \rightarrow \mathcal{P}(X) : S \mapsto \begin{cases} \overline{S(i)} & \text{if } S(i) \subseteq [i-j, i] \\ S(i) & \text{otherwise.} \end{cases}$$

For example for the  $k = 6, 8$  the map  $\phi_1^2$  is indicated by a vertex in Figure 5(i) and (ii), respectively.

To establish the next result, we associated to every element  $i \in X$  the split systems  $\Sigma(i)^+ := \{S \in \Sigma_k : S(i+1) = S(i) \neq S(i-1)\}$ . Then the partial ordering “ $\preceq_i$ ” defined, for all  $S, S' \in \Sigma_k$ , by putting  $S \preceq_i S'$  if  $|S(i)| \leq |S'(i)|$ , is clearly a total ordering of  $\Sigma(i)^+$  with minimal element  $S_i^+ = [i, i+1]|X - [i, i+1]$

**Lemma 5.1.** *For any  $k \geq 4$  the following statements hold:*

- (i) *For all  $i \in \{1 \dots, k\}$  and all  $0 \leq j < k-3$  the map  $\phi_i^j$  is a vertex of  $G(\Sigma_k)$ ,  $\phi_i^{k-3} = \phi_{i+1}^0$  holds, and  $\Delta(\phi_i^j, \phi_i^{j+1}) = \{[i-j-1, i]|X - [i-j-1, i]\}$ . In particular,  $\{\phi_i^j, \phi_i^{j+1}\}$  is an edge in  $G(\Sigma_k)$ .*
- (ii) *For all  $i \in \{1 \dots, k\}$  and all  $1 \leq j < k-3$ , the map*

$$\psi_i^j : \Sigma_k \rightarrow \mathcal{P}(X) : S \mapsto \begin{cases} \overline{\phi_i^j(S)} & \text{if } S = S_i^+ \\ \phi_i^j(S) & \text{otherwise.} \end{cases}$$

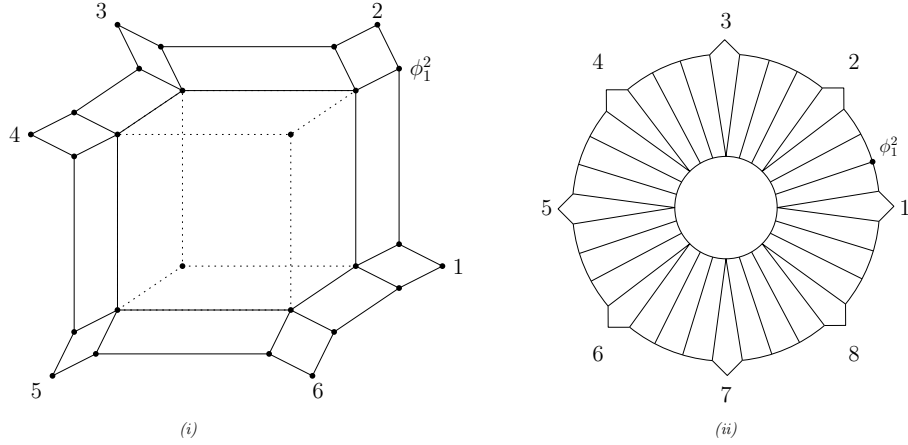


Figure 5: For  $k = 6$ , we depict in (i) the Buneman graph  $G(\Sigma_6)$  in terms of bold and dashed edges and the associated 6-marguerite  $M(\Sigma_6)$  in terms of bold lines. In addition we indicated the vertex  $\phi_1^2$  of  $G(\Sigma_6)$ . We picture the 8-marguerite in (ii) and indicate again the vertex  $\phi_1^2$ .

is a vertex in  $G(\Sigma_k)$  that is adjacent with  $\phi_i^j$ . Moreover  $\psi_i^{k-3} = \psi_{i+1}^0$  and  $\{\psi_i^j, \psi_i^{j+1}\}$  is an edge in  $G(\Sigma_k)$ .

*Proof.* (i) Suppose  $i \in \{1, \dots, k\}$  and  $0 \leq j < k-3$ . To see that  $\phi_i^j \in V(\Sigma_k)$ , we distinguish between the cases that (a)  $j = 0$ , (b)  $j = k-3$ , and (c)  $1 \leq j \leq k-4$ . Let  $i \in \{1, \dots, k\}$ .

Assume first that (a) holds and let  $S \in \Sigma_k$ . Then  $\phi_i^0(S) = S(i)$  must hold since  $\Sigma_k$  does not contain trivial splits. Moreover,  $\phi_i^0(S) = \overline{S(i)}$  holds if and only if  $S(i) \subseteq \{i\}$  if and only if  $S$  is the trivial split  $i|X-i$ . Thus,  $\phi_i^0$  is a vertex in  $G(\Sigma_k)$  in this case.

Assume next that (b) holds. We claim that  $\phi_i^{k-3} = \phi_{i+1}^0$ . Assume again that  $S \in \Sigma_k$ . Observe that since  $i - (k-3) \equiv i+3 \pmod{k}$  we have  $S(i) \subseteq \{i - (k-3), \dots, i\}$  if and only if  $\{i+1, i+2\} \subseteq \overline{S(i)}$ . We distinguish the cases that (α)  $S(i) = S(i+1)$  and (β)  $S(i) \neq S(i+1)$ .

Assume first that Case (α) holds, that is,  $S(i) = S(i+1)$ . Then  $\{i+1, i+2\} \not\subseteq \overline{S(i)}$ . Combined with the observation made at the beginning of the proof of this case, we obtain  $S(i) \not\subseteq \{i - (k-3), \dots, i\}$  and, so,  $\phi_i^{k-3}(S) = S(i) = S(i+1) = \phi_{i+1}^0(S)$ .

Next, assume that Case (β) holds, that is,  $S(i) \neq S(i+1)$ . Then  $i+1 \in \overline{S(i)}$ . Since  $S$  cannot be a trivial split it follows that  $i+2 \in \overline{S(i)}$  must hold too. Combined again with the observation made at the beginning of the proof of this case, it follows that  $S(i) \subseteq \{i - (k-3), \dots, i\}$ . Thus,  $\phi_i^{k-3}(S) = \overline{S(i)} = S(i+1) = \phi_{i+1}^0(S)$  which completes the proof of the claim. In combination with Case (α),  $\phi_i^{k-3} \in G(\Sigma_k)$  follows.

So assume that (c) holds. Combining (a) with (Bii) and the fact that  $\phi_i^0(S) = \phi_i^1(S)$  for all  $S \in \Sigma_k - \{S_i^+\}$  and  $\phi_i^0(S_i^+) = \overline{\phi_i^1(S_i^+)}$ , it follows that  $\phi_i^1$  is a vertex

of  $G(\Sigma_k)$ . Similar arguments imply that if  $\phi_i^l$  is a vertex in  $G(\Sigma_k)$  then so is  $\phi_i^{l+1}$ . This concludes the proof of Case (c).

That  $\Delta(\phi_i^j, \phi_i^{j+1}) = \{[i-j-1, i] | X - [i-j-1, i]\}$  holds for all  $i \in \{1 \dots, k\}$  and  $0 \leq j < k-3$  is an immediate consequence of the construction.

(ii) Suppose  $i \in \{1 \dots, k\}$  and  $1 \leq j < k-3$ . Then  $\psi_i^j$  must be a vertex of  $G(\Sigma_k)$  that is adjacent with  $\phi_i^j$  in view of (Bii) as  $S_i^+ \in \Sigma^{\phi_i^j}$ . That  $\psi_i^1 = \psi_{i-1}^{k-3}$  is implied by the fact that the two splits in which  $\psi_i^{k-3}$  and  $\psi_{i+1}^1$  differ from  $\phi_{i+1}^0$  are incompatible. That  $\{\psi_i^j, \psi_i^{j+1}\}$  is an edge in  $G(\Sigma_k)$  follows from the fact that  $\{\phi_i^j, \phi_i^{j+1}\}$  is an edge in  $G(\Sigma_k)$ .  $\square$

Bearing in mind Lemma 5.1, we next associate to  $G(\Sigma_k)$  the  $k$ -marguerite  $M(\Sigma_k)$  on  $X$ , that is, the subgraph of  $G(\Sigma_k)$  induced by the set of maps  $\phi_i^j$  and  $\psi_i^l$  where  $1 \leq i \leq k$ ,  $0 \leq j < k-3$  and  $1 \leq l < k-3$ . We illustrate this definition for  $k = 6, 8$  in Fig. 5. Note that if  $k$  or  $X$  are of no relevance to the discussion then we will also refer to a  $k$ -marguerite on  $X$  simply as a *marguerite*.

Clearly,  $G(\Sigma_k)$  and  $M(\Sigma_k)$  coincide for  $k = 4, 5$ . To be able to shed light into the structure of  $k$ -marguerites for  $k \geq 6$ , we require some more terminology. Suppose  $k \geq 4$  and  $i \in \{0, \dots, k\}$ . Then we call a vertex of  $M(\Sigma_k)$  of the form  $\phi_i^0$  an *external vertex*. Moreover, we call for all  $0 \leq j < k-3$  an edge of  $M(\Sigma_k)$  of the form  $\{\phi_i^j, \phi_i^{j+1}\}$  an *external edge*. Note that since  $M(\Sigma_k)$  is in particular a subgraph of the  $|\Sigma_k|$ -dimensional hypercube, any split in  $\Sigma_k$  not of the form  $i, i+1 | X - \{i, i+1\}$  is Bu-displayed in terms of four parallel edges of  $M(\Sigma_k)$  exactly two of which are external.

## 5.2. Gates

In this section we establish that any partially-resolved 1-nested network can be embedded into the Buneman graph associated to  $\Sigma(N)$  thus allowing the bringing to bear of a wealth of results for the Buneman graph to such networks. Of particular interest to us are gated subsets of  $V(\Sigma)$  where a subset  $Y \subseteq Z$  of a (proper) metric space  $(Z, D)$  is called a *gated* subset of  $Z$  if there exists for every  $z \in Z$  a (necessarily unique) element  $y_z \in Y$  such that  $D(y, z) = D(y, y_z) + D(y_z, z)$  holds for all  $y \in Y$ . We refer to  $y_z$  as the *gate* for  $z$  in  $Y$ .

We start with associating a metric space to the Buneman graph of a split system. Suppose  $\Sigma$  is a split system on  $X$  such that for all  $x$  and  $y$  in  $X$  distinct there exists some  $S \in \Sigma$  such that  $S(x) \neq S(y)$ . Then the map  $D : V(\Sigma) \times V(\Sigma) \rightarrow \mathbb{R}_{\geq 0} : (\phi, \phi') \mapsto |\Delta(\phi, \phi')|$ , is a (proper) metric on  $V(\Sigma)$  (see e.g. [14, page 52]) that is,  $D$  attains 0 only on the main diagonal, is symmetric, and satisfies the triangle inequality.

For  $\Sigma$  a split system on  $X$  and  $\Sigma' \in \pi_0(\Sigma)$ , the following two additional properties of the Buneman graph will be useful.

(Bvi) The map

$$V(\Sigma') \rightarrow V(\Sigma) : \phi \mapsto (\tilde{\phi} : \Sigma \rightarrow \mathcal{P}(X) : S \mapsto \begin{cases} \phi(S) & \text{if } S \in \Sigma', \\ \max(S|\Sigma') & \text{otherwise} \end{cases})$$

is an isometry between  $G(\Sigma')$  and the block  $B(\Sigma')$  of  $G(\Sigma)$ .

(Bvii) For every map  $\phi \in V(\Sigma)$ , the map  $\phi_{\Sigma'}$  given by

$$\phi_{\Sigma'} : \Sigma(N) \rightarrow \mathcal{P}(X) : S \mapsto \begin{cases} \phi(S) & \text{if } S \in \Sigma' \\ \max(S|\Sigma') & \text{otherwise,} \end{cases}$$

is the gate for  $\phi$  in  $B(\Sigma')$ . We denote by  $Gates(G(\Sigma))$  the set of all vertices  $\phi$  of  $G(\Sigma)$  for which there exists a block  $B \in \mathfrak{Bl}(G(\Sigma))$  such that  $\phi$  is the gate for some  $x \in X$  in  $B$ .

**Lemma 5.2.** *Suppose  $N$  is a 1-nested network on  $X$ . Then a block of  $G(\Sigma(N))$  is either a cut-edge or contains precisely one marguerite. Moreover the gates of a marguerite  $M$  in  $G(\Sigma(N))$  are the maps  $\tilde{\phi}$  where  $\phi$  is an external vertex of  $M$ .*

*Proof.* Suppose  $\Sigma' \in \pi_0(\Sigma(N))$ . Note that  $|\Sigma'| = 1$  if and only if  $B(\Sigma')$  is a cut-edge of  $G(\Sigma(N))$ . So assume that  $|\Sigma'| \geq 2$ . Then  $B(\Sigma')$  is a block of  $G(\Sigma(N))$  and, so, there exists a unique cycle  $C$  of  $N$  of length  $k \geq 4$  such that  $\Sigma(C) = \Sigma'$ . Let  $Y$  denote the partition of  $X$  induced by deleting all edges of  $C$  and let  $\Sigma'_Y$  denote the split system on  $Y$  induced by  $\Sigma(C)$ . Then  $\Sigma'_Y$  is of the form  $\Sigma_k$  and, so,  $G(\Sigma'_Y)$  contains the  $k$ -marguerite  $M(\Sigma'_Y)$ . Combined with Property (Bvi) it follows that  $G(\Sigma(N))$  contains the marguerite  $M(\Sigma'_Y)$  (or, more precisely, the graph obtained by replacing for every external vertex  $\phi_i^0$ ,  $1 \leq i \leq k$ , the label  $Y_i \in Y$  by the elements in  $Y_i$ ).

To see the remainder of the lemma suppose that  $M$  is a marguerite and assume that  $k \geq 4$  such that  $M = M(\Sigma_k)$ . Let  $Y = \{X_1, \dots, X_k\}$  denote the partition of  $X$  induced by  $\Sigma_k$  and assume that  $x \in X$ . Then there must exist some  $i \in \{1, \dots, k\}$  such that  $x \in X_i$ . Since  $\phi_i^0$  is clearly the map

$$\phi_i^0 : \Sigma_k \rightarrow \mathcal{P}(X) : S = A|B \mapsto \begin{cases} A & \text{if } X_i \subseteq A \\ B & \text{if } X_i \subseteq B, \end{cases}$$

Properties (Bvi) and (Bvii) imply that  $\tilde{\phi}_i^0$  is the gate for  $x$  in  $M$ .  $\square$

To be able to establish that any 1-nested partially resolved network  $N$  can be embedded as a (not necessarily induced) subgraph into the Buneman graph  $G(\Sigma(N))$  associated to  $\Sigma(N)$ , we require again more terminology. Suppose  $N$  is a partially-resolved 1-nested network and  $v$  is a non-leaf vertex of  $N$ . Then  $v$  is either incident with three or more cut-edges of  $N$ , or there exists a cycle  $C_v$  of  $N$  that contains  $v$  in its vertex set. In the former case, we choose one of them and denote it by  $e_v$ . In addition, we denote by  $x_v \in X$  an element such that  $e_v$  is not contained in any path in  $N$  from  $x_v$  to  $v$ . In the latter case, we define  $x_v$  to be an element in  $X$  such that no edge of  $C_v$  is contained in any path in  $N$  from  $v$  to  $x_v$ .

**Theorem 5.3.** *Suppose  $N$  is a 1-nested partially-resolved network on  $X$ . Then the map  $\psi : V(N) - X \rightarrow Gates(G(\Sigma(N)))$  defined by mapping every non-leaf vertex  $v \in V(N)$  to the map*

$$\xi(v) : \Sigma(N) \rightarrow \mathcal{P}(X) : S \mapsto \begin{cases} \max(S|\Sigma^*) & \text{if } S \in \Sigma(N) - \Sigma^* \\ S(x_v) & \text{else} \end{cases}$$

is a bijection between the set of non-leaf vertices of  $N$  and the gates of  $G(\Sigma(N))$  where  $\Sigma^* = \{S_{e_v}\}$  if  $v$  is contained in three or more cut-edges of  $N$  and  $\Sigma^* = \Sigma(C_v)^-$  else. In particular,  $\xi$  induces an embedding of  $N$  into  $G(\Sigma(N))$  by mapping each leaf  $x$  of  $N$  to the leaf  $\phi_x$  of  $G(\Sigma(N))$  and replacing for any two adjacent vertices  $v$  and  $w$  of a cycle  $C$  of  $N$  of length  $k$  the edge  $\{v, w\}$  by the path  $\phi_i^0 := \xi(v), \phi_i^1, \dots, \phi_i^{k-3} := \xi(w)$ .

*Proof.* Suppose  $N$  is a 1-nested network and put  $\Sigma = \Sigma(N)$ . To see that  $\xi$  is well-defined suppose  $v \in V(N) - X$ . Then  $v$  is either contained in three or more cut-edges of  $N$  or  $v$  is a vertex of some cycle  $C$  of  $N$ . In the former case we obtain  $\{S_{e_v}\} \in \pi_0(\Sigma(N))$  and in the later we have  $C = C_v$  and  $\Sigma(C_v)^- \in \pi_0(\Sigma)$ . In either case, the definition of the element  $x_v$  combined with Property (Bvii) implies  $\xi(v) \in \text{Gates}(G(\Sigma))$ .

To see that  $\xi$  is injective suppose  $v$  and  $w$  are two non-leaf vertices of  $N$  such that  $\xi(v) = \xi(w)$ . Assume for contradiction that  $v \neq w$ . It suffices to distinguish between the cases that (i)  $v$  and  $w$  are contained in the same cycle, and that (ii) there exists a cut edge  $e'$  on any path from  $v$  to  $w$ .

To see that (i) cannot hold, suppose that  $v$  and  $w$  are vertices on a cycle  $C$  of  $N$ . Then,  $S(x_v) = \max(S|\Sigma(C)^-) = S(x_w)$  must hold for the m-split  $S$  obtained by deletion of the two edges of  $C$  adjacent to  $v$  which is impossible. Thus (ii) must hold. Hence, there must exist a cut-edge  $e'$  on the path from  $v$  to  $w$ . Then  $\xi(v)(S_{e'}) \neq \xi(w)(S_{e'})$  follows which is again impossible. Thus,  $\xi$  must be injective.

To see that  $\xi$  is surjective suppose  $g \in \text{Gates}(G(\Sigma))$ . Then there exists some  $x_g \in X$  and some block  $B \in \mathfrak{Bl}(G(\Sigma))$  such that  $g$  is the gate for  $x_g$  in  $B$ . Let  $\Sigma_B \in \pi_0(\Sigma(N))$  denote the connected component that, in view of Property (Bv) is in one-to-one correspondence with  $B$ . If there exists a cycle  $C$  of  $N$  such that  $\Sigma(C)^- = \Sigma_B$  then let  $v_g$  be a vertex of  $N$  such that no edge on any path from  $v_g$  to  $x_g$  crosses an edge of  $C$ . Then, by construction,  $\xi(v_g) = g$ . Similar arguments show that  $\xi(v_g) = g$  must hold if  $\Sigma_B$  contains precisely one split and thus corresponds to a cut-edge of  $N$ . Hence,  $\xi$  is also surjective and thus bijective.

The remainder of the theorem is straight-forward.  $\square$

Theorem 5.3 implies that by carrying out steps (Ci) and (Cii) stated in Corollary 5.4 any 1-nested partially-resolved network  $N$  induces a 1-nested network  $N(\Sigma(N))$  such that split system  $\Sigma(N(\Sigma(N)))$  induced by  $N(\Sigma(N))$  is the split system  $\Sigma(N)$  induced by  $N$ .

**Corollary 5.4.** *Let  $\Sigma$  be a split system on  $X$  for which there exists a 1-nested network  $N$  such that  $\Sigma = \Sigma(N)$ . Then we can obtain  $N(\Sigma)$  from  $G(\Sigma)$  by carrying out steps (Ci) and (Cii):*

(Ci) *For all  $x \in X$  replace each leaf  $\phi_x$  by  $x$ , and*

(Cii) *For all blocks  $B$  of  $G(\Sigma)$  that contain a  $k$ -marguerite  $M$  for some  $k \geq 4$ , first add the edges  $\{\phi_i^0, \phi_{i+1}^0\}$  for all  $i \in \{1, \dots, k\}$  where  $k+1 := 1$  and then delete all edges and vertices of  $B$  not of the form  $\phi_i^0$  for some  $1 \leq i \leq k$ .*



We next show that even if the circular split system under consideration does not satisfy the assumptions of Corollary 5.4, steps (Ci) and (Cii) still give rise to a, in a well-defined sense, optimal 1-nested network

**Theorem 5.5.** *Let  $\Sigma$  be a circular split system on  $X$  that contains all trivial splits on  $X$ . Then  $N(\Sigma)$  is a 1-nested network such that:*

- i)  $\Sigma \subseteq \Sigma(N)$ ,
- ii)  $|\Sigma(N)|$  is minimal among the 1-nested network satisfying i),
- iii) A vertex  $v$  of a cycle  $C$  of  $N$  is partially resolved if and only if the split displayed by the edges of  $C$  incident with  $v$  belongs to  $\Sigma$ .

Moreover  $N$  is unique up to isomorphism and partial-resolution.

*Proof.* (i) & (ii): Suppose for contradiction that there exists a 1-nested network  $N'$  such that  $\Sigma \subseteq \Sigma(N')$  and  $|\Sigma(N')| < |\Sigma(N(\Sigma))|$ . Without loss of generality, we may assume that  $N'$  is such that  $|\Sigma(N')|$  is as small as possible. Moreover, we may assume without loss of generality that  $N'$  and  $N(\Sigma)$  are both maximal partially-resolved. To obtain the required contradiction, we employ Corollary 4.8 to establish that  $N'$  and  $N(\Sigma)$  are isomorphic.

Since  $\Sigma \subseteq \mathcal{I}(\Sigma)$  it is clear that  $\mathcal{I}(\Sigma)$  contains all trivial splits of  $X$ . Furthermore, since  $\Sigma$  is circular, Corollary 3.4(i) implies that  $\mathcal{I}(\Sigma)$  is circular. Since  $\mathcal{I}(\Sigma)$  is clearly  $\mathcal{I}$ -intersection closed and, by Property (Bi),  $\mathcal{I}(\Sigma)$  is the split system Bu-displayed by  $G(\mathcal{I}(\Sigma))$  it follows that  $\mathcal{I}(\Sigma)$  comprises all splits displayed by  $N(\mathcal{I}(\Sigma))$ . Hence, by Corollary 4.8, up to isomorphism and partial-resolution,  $N(\mathcal{I}(\Sigma))$  is the unique 1-nested network for which the displayed split system is  $\mathcal{I}(\Sigma)$ .

We claim that  $\mathcal{I}(\Sigma) = \Sigma(N')$  holds too. By Corollary 3.4(iii), we have  $\mathcal{I}(\Sigma) \subseteq \Sigma(N')$ . To see the converse set inclusion assume that  $S \in \mathcal{I}(\Sigma)$ . Then  $S$  is either induced by (a) a cut-edge of  $N'$  or (b)  $S$  is not an m-split and there exists a cycle  $C$  of  $N'$  that displays  $S$ . In case of (a) holding,  $S \in \Sigma$  follows by the minimality of  $|\Sigma(N')|$ . So assume that (b) holds. Then there must exist some connected component  $\Sigma_C \in \pi_0(\Sigma)$  that displays  $S$ . Hence, by Property (Bv), there exists some block  $B_C \in \mathfrak{BI}(\Sigma)$  such that the split system Bu-displayed by  $B_C$  is  $\Sigma_C$ . Hence,  $\Sigma_C$  is also displayed by  $N(\Sigma)$ . Since, as observed above  $\Sigma(N(\Sigma)) = \mathcal{I}(\Sigma)$  we also have  $\Sigma(N') \subseteq \mathcal{I}(\Sigma)$  the claim follows.

(iii) Suppose  $C$  is a cycle of  $N$  and  $v$  is a vertex of  $C$ . Assume first that  $v$  is partially resolved. Then there exists a cut-edge  $e$  of  $N$  that is incident with  $v$ . Note that the split  $S_e$  displayed by  $e$  is also displayed by the two edge of  $C$  incident with  $v$ . In view of Property (Bi) and, implied by (Ci) and (Cii), that the cut-edges of  $N$  are in 1-1 correspondence with the cut-edges of  $G(\Sigma)$  we obtain  $S_e \in \Sigma$ .

To see the converse assume that  $e_1$  and  $e_2$  are the two edges of  $C$  incident with  $v$  such that the split  $S$  displayed by  $\{e_1, e_2\}$  is contained in  $\Sigma$ . Then  $S$  is compatible with all splits in  $\Sigma - \{S\}$ . By Property (Bv), it follows that there exists a cut-edge  $e$  in  $G(\Sigma)$  such that  $S_e = S$ . Combined with (Ci) and (Cii) it follows that  $v$  is partially resolved.  $\square$

## 6. Open Questions

In this paper, we have started to investigate the interplay between Buneman graphs and 1-nested networks. Although our results are encouraging involving non-trivial characterizations, numerous questions that might be of interest have remained unanswered. For example, regarding Corollary 4.8 what is the minimal size of  $\Sigma$  that allows one to, in our sense, uniquely recover  $\Sigma(N)$ ? Also, is it possible to characterize split system induced by level-2 networks (i.e. networks obtained from level-1 networks by adding a cord to a cycle)? Finally, a number of reconstruction algorithms to reconstruct rooted level-1 networks try and infer them from a collection rooted binary phylogenetic trees on three leaves. Such trees are generally referred to as triplets and in real biological studies it is generally too much to hope for that a set of triplets contains *all* triplets induced by the (unknown) underlying network. One way to overcome this problem is to employ triplet inference rules. Such rules are well-known for rooted phylogenetic trees but are missing for general level-1 networks. The question therefore becomes if the work presented here combined with results on closure obtained in [19] might provide a starting point for developing such rules.

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